mathematics

MDPI

Article

Weighted Asymmetry Index: A New Graph-Theoretic Measure for Network Analysis and Optimization

Ali N. A. Koam [1], Muhammad Faisal Nadeem [2,*], Ali Ahmad [3] and Hassan A. Eshaq [4]

[1] Department of Mathematics, College of Science, Jazan University, P.O. Box 114, Jazan 45142, Saudi Arabia; akoum@jazanu.edu.sa
[2] Department of Mathematics, COMSATS University Islamabad, Lahore Campus, Lahore 54000, Pakistan
[3] Department of Computer Science, College of Engineering and Computer Science, Jazan University, Jazan 45142, Saudi Arabia; aimam@jazanu.edu.sa
[4] Department of Educational Sciences, Faculty of Arts and Humanities, Jazan University, Jazan 45142, Saudi Arabia; haeshaq@jazanu.edu.sa
* Correspondence: mfaisalnadeem@ymail.com

Abstract: Graph theory is a crucial branch of mathematics in fields like network analysis, molecular chemistry, and computer science, where it models complex relationships and structures. Many indices are used to capture the specific nuances in these structures. In this paper, we propose a new index, the weighted asymmetry index, a graph-theoretic metric quantifying the asymmetry in a network using the distances of the vertices connected by an edge. This index measures how uneven the distances from each vertex to the rest of the graph are when considering the contribution of each edge. We show how the index can capture the intrinsic asymmetries in diverse networks and is an important tool for applications in network analysis, optimization problems, social networks, chemical graph theory, and modeling complex systems. We first identify its extreme values and describe the corresponding extremal trees. We also give explicit formulas for the weighted asymmetry index for path, star, complete bipartite, complete tripartite, generalized star, and wheel graphs. At the end, we propose some open problems.

Keywords: weighted asymmetry index; network analysis; distance-based indices; optimization; complex systems; asymmetry in networks

MSC: 05C82; 05C12; 90C27

check for updates

Citation: Koam, A.N.A.; Nadeem, M.F.; Ahmad, A.; Eshaq, H.A. Weighted Asymmetry Index: A New Graph-Theoretic Measure for Network Analysis and Optimization. *Mathematics* **2024**, *12*, 3397. https://doi.org/10.3390/math12213397

Academic Editor: Andrea Scozzari

Received: 26 September 2024
Revised: 25 October 2024
Accepted: 29 October 2024
Published: 30 October 2024

Copyright: © 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https://creativecommons.org/licenses/by/4.0/).

1. Introduction

Graph theory is one of the basic and essential sections of mathematics, which, in its turn, has found numerous applications in different branches of science. As for computer science, it is one of the key instruments applied in the context of designing and analyzing algorithms; most importantly, it is applied in the field of networking, where graphs model connections between nodes in the internet or social graphs [1,2]. In the field of biology, graph theory is useful in revealing complex networks such as food webs, protein interactions, and mapping genomes [3]. As a result, it allows an understanding of biological processes and evolution. The domain in which graph theory is applied within the chemistry field is mainly the modeling of molecular structures [4,5], with atoms described as vertices and bonds as edges, to aid in predicting the properties and reactions of chemicals. In physics, too, the theory is applied to particle interactions and quantum states, where complex networks describe the relations of different elements [6].

Furthermore, graph theory has been widely applied in transportation [7] and logistics to optimize routes for cost reductions [8], thus enhancing efficiency; it is used to model road networks and supply chains. The social sciences have used it for research on social networks [9]. It gives the ability to find relationships between people or visualize the

spread of information or diseases. Generally, graph theory is ubiquitous and can be applied across scientific areas as a foundation for researchers to model, analyze, and solve difficult problems.

A topological index is a numerical value that characterizes the graph's structure and remains invariant to any different isomorphism of the graph. The most important application of such indices is in the study of molecular structures [10], especially in chemistry, where the properties of the behavior of other kinds of chemicals can be predicted using them. Topological indices, based on molecular graph representation, encompass features at various levels of description that range from connectivity to symmetry and provide a relationship with the physical and chemical properties of the molecule, such as boiling points, stability, and reactivity. Topological indices find applications not only in the field of chemistry. They are used to help design new materials with desired properties in material science by predicting how changes in structure might affect material behavior. Within pharmacology, these indices help design drugs by enabling the comparison of molecular structures of possible drug candidates with optimum biological activity [11,12]. In the theory of networks, it is possible to apply topological indices for analyzing robustness and efficiency with respect to the possible optimization of the design and function of networks, whatever the context: whether related to telecommunications, social, or transportation system studies [13–15]. Therefore, topological indices are some of the powerful tools in quite diverse scientific and engineering disciplines. In physics, topological indices are used to analyze the resistance and energy dissipation in electrical networks, as well as to study vibrational modes in molecular structures [16,17]. They help quantify the robustness and efficiency of physical systems modeled as graphs.

Distance-based indices are defined to capture the relational properties of a graph by considering the distances between pairs of vertices. Such indices can elaborate on graph structure properties beyond simple connectivity and allow for the nature of elements' spatial relations with each other in the graph to be much more elaborately explained. In chemistry, distance-based topological descriptors are important in predicting certain molecular properties, like boiling points [18], stability [19], and reactivity to biological activity [20]. For more applications, see [21,22]. Distance-based indices consider how atoms are positioned relative to each other within a molecule. In network analysis, these same indices contribute to the assessment of the efficiency of communication paths, the optimization of routing protocols, and the evaluation of the vulnerability of networks to disruptions. Their ability to quantify intricate, often relational, structures renders them invaluable tools across many scientific and engineering applications.

Due to their vast uses and applications, many researchers are working on the properties and their uses in different fields. Zhang et al. use topological indices to study anti-malaria drugs [23]. Ullah finds the topological indices for 2-D nanotubes [24]. Gutman et al. introduce a geometric method for constructing vertex-degree-based molecular structure descriptors using an ellipse model [25]. Hayat et al. investigate the effectiveness of temperature-based graphical indices in predicting the thermodynamic properties of benzenoid hydrocarbons through QSPR modeling [26]. Huang et al. examine the use of degree-based topological indices to analyze the structural properties of drugs used to treat Lyme disease [27]. Arockiaraj et al. address the challenges in drug development—such as time consumption, cost, safety profiles, and inadequate experimental data—by leveraging chemical graph theory to analyze molecular structures through topological indices [28]. Ghani et al. explore the use of distance-based entropy in analyzing chemical structures, with a particular focus on polyphenylenes and boron (B12) [29]. Doslic et al. define a new topological index, the Mostar index [30]. Zaman et al. focus on deriving mathematical expressions for resistance distance-based topological indices within four specific families of graph networks, where edges represent unit resistors in an electrical network [31]. Nagarajan et al. apply topological indices, derived from the molecular graphs of key drugs like lopinavir, ritonavir, arbidol, thalidomide, chloroquine, hydroxychloroquine, theaflavin, and remdesivir, in the fight against COVID-19 [32].

Gao et al. [33] discuss the differences imposed between Mostar index and irregularity in graphs, giving an in-depth study of the mathematical properties and their relations. Havare [34] studied Mostar index and edge Mostar index concerning different cycle-related graphs. The Wiener index is defined as a well-known topological index, which includes the summation of the shortest path distances between every pair of vertices in a graph. Dinar et al. [35] extended the concept of the Wiener index to intuitionistic fuzzy graphs and showed its application on an optimization problem dealing with a water pipeline network. Similarly, Asmarani et al. 2023 [36] discuss the Wiener index together with the first Zagreb index and the Gutman index in terms of the power of dihedral groups. PI index is another important topological descriptor, whose estimation has been widely studied owing to its applicability in chemical graph theory. Khadikar et al. [37] studied the PI index of polyacenes, which is an important class of organic compounds. Ilić and Milosavljević extend the PI index by proposing the weighted vertex PI index, considering the incorporation of weights at vertices within the framework of the PI index [38]. Betweenness centrality is one of the important measures in network analysis, which quantifies the role of vertices regarding their potential to facilitate communication in the network. Barthelemy [39] considers betweenness centrality in large complex networks, and discusses some computational aspects and provides an insight into the role it plays in understanding resilience versus efficiency in a network.

2. Motivation

The weighted asymmetry index is a graph-theoretic measure introduced in this paper based on the limitations that exist in distance-based and centrality-based indices such as the Wiener index [40], Szeged index [41], PI index [42], Mostar index [30], and centrality measures such as betweenness centrality [43], stress centrality [44], decay centrality [45], and the Shimbel index [46]. These traditional indices have widely been used for quantifying the properties of graphs, such as distances between pairs of vertices, the influence of nodes, and centrality within a network. However, beyond their wide popularity and usefulness, these indices cannot capture the finer structural asymmetries common in many complex networks.

The well-known distance-based topological indices such as the Wiener index and the Szeged index have played an important role in structuring graphs. They calculate the summation of distances between all pairs of vertices in a graph. Applications range from the prediction of various important properties of molecules to the diagnosis of network performances. However, they treat every pair of vertices equally and do not differentiate symmetric from asymmetric structures. Considering the critical aspect of local imbalances or asymmetric vertex distribution, in social networks or structures of a molecular nature, for instance, the Wiener index perhaps depends too much on an oversimplification of the structural properties of the graph. The Szeged index refines the Wiener index by including in it edge-based vertex distances. In this way, it considers the number of vertices on either side of an edge, entailing a layer of local analysis in addition to the global distance measure. Still, however, the Szeged index cannot capture the asymmetry in detail between connected vertices in those graphs where edge weights or local imbalances carry valuable information about the function of the network. The Mostar index defines the peripherality measure quantifying the imbalance in the number of vertices closer to one end of an edge compared to the other. This index captures some level of asymmetry; still, it suffers from very low sensitivity about weighted or distance-related asymmetry, which could be essential in the analysis of either molecular stability or network vulnerability.

Examples of measures based on centrality include betweenness centrality, stress centrality, and decay centrality. Centrality metrics can provide information about the influence and importance of vertices within a graph. For example, betweenness centrality will be able to measure the number of times a node will lie on the shortest path between other nodes; hence, this metric is useful for finding the most vital nodes in a network concerning communication or flow in a social network. These metrics do not consider the relative distances

or asymmetry between neighboring vertices. This is a serious limitation when working in domains where local structural imbalances may affect network performance, as in transportation networks with uneven node distributions or molecular interaction networks.

The weighted asymmetry index assigns weights to any pair of distances between vertices and edges according to their relative importance or influence within the structure and denotes these as WA. Unlike more 'traditional' indices, which are based on any form of distance, the WA index differentiates between vertices about their local context with regard to capturing the asymmetry in connectivity and influence. This makes for a more sensitive and exact measure of structural imbalance, which might render the WA index especially useful in those analyses of graphs where local asymmetries may play a critical role in the overall network behavior. For example, in the field of molecular chemistry, structural imbalances with respect to atom distances affect both the stability and reactivity of molecules. The WA index, considering weighted distances, can predict such properties more precisely than, for instance, the Wiener or Szeged indices do. In studies on network resilience, like communication or transportation studies, asymmetric structures bring about vulnerabilities. Application of the WA index identifies nodes or edges that disproportionately affect network stability due to their asymmetric connectivity.

3. Basic Definitions and Known Results

Below are some essential notations, definitions, and references from the literature that are crucial for understanding our main results.

Definition 1. *A simple graph $G = (V, E)$ is an undirected graph consisting of the following:*

- *A finite set V of vertices.*
- *A set E of edges, where each edge is an unordered pair $\{u, v\}$, with $u, v \in V$ and $u \neq v$ (i.e., no loops are allowed). Additionally, there are no multiple edges between any pair of vertices.*

Definition 2. *The order of a graph G is the number of vertices $|V|$, and the size is the number of edges $|E|$.*

Definition 3. *The distance between two vertices u and v in a graph G is the length of the shortest path connecting them, denoted $d(u, v)$.*

Definition 4. *Given an edge $e = uv$ in a graph G, the value $\theta_u(e)$ is defined as the number of vertices in G that are closer to vertex u than to vertex v.*

Definition 5. *The term $\widetilde{C_v}$ is defined as*

$$\widetilde{C_v} = \sum_{w \in V(G)} \frac{1}{d(v, w) + 1}.$$

The most commonly used distance-based indices in network characterization have indicative purposes of distances between vertices. Distance-based topological indices play an important role in structure–property and structure–activity studies, which enable them to predict the biological activity of chemical compounds. The first distance-based index was proposed by Wiener [40], known as the Wiener index. It is defined as

$$W(G) = \sum_{u,v \in V(G)} d(u, v).$$

Independently, Plavšić et al. [47] and Ivanciuc et al. [48] proposed the Harary index, which is calculated as the sum of the reciprocals of shortest path distances between all pairs of vertices. The hyper-Wiener index, as a generalization of the Wiener index, includes

the sum of all distances and the sum of the squares of these distances between all vertex pairs [49]:

$$WW(G) = \frac{1}{2}\sum_{u\neq v}(d(u,v) + d(u,v)^2).$$

The Szeged index (Sz(G)) is defined for each edge $e = (u,v)$ as the product of the number of vertices closer to u and the number of vertices closer to v (including u and v themselves). The index sums this product over all edges [41]:

$$Sz(G) = \sum_{e=(u,v)\in E(G)} \theta_u(e)\cdot\theta_v(e).$$

The PI index is a distance-based index closely related to the Szeged index [42]. It is computed by summing the differences between the number of vertices closer to one endpoint of an edge than the other:

$$PI(G) = \sum_{e=(u,v)\in E(G)} (\theta_u(e) + \theta_v(e)).$$

The Mostar descriptor is given by [30]

$$Mo(G) = \sum_{uv\in E(G)} |\theta_u - \theta_v|.$$

In addition to topological indices, distance-based indices can also be found in other areas of graph theory and network analysis. These indices typically focus on aspects of graph structure, centrality, or even dynamic processes in graphs.

Betweenness centrality is a measure of how many shortest paths between all pairs of other nodes pass through a given node v [43]. It indicates how critical a vertex is in controlling the flow of information or connectivity in a graph.

$$C_B(v) = \sum_{s\neq v\neq t} \frac{\sigma_{st}(v)}{\sigma_{st}},$$

where σ_{st} represents the total number of shortest paths between vertex s and vertex t, while $\sigma_{st}(v)$ denotes the number of those paths that pass through vertex v.

Stress centrality is defined as the sum of all the shortest paths passing through a vertex v, taken over all ordered pairs of vertices [44]. Unlike betweenness centrality, it considers all paths and is not normalized by the total number of shortest paths.

$$S(v) = \sum_{s\neq v\neq t} \sigma_{st}(v).$$

Decay centrality considers the influence of a vertex v on other vertices, with the influence decaying with distance [45], and is defined as

$$C_D(v) = \sum_{u\in V(G)} \delta^{d(v,u)}.$$

The symbol $\delta^{d(v,u)}$ in the context of decay centrality represents the decayed influence that vertex v has on vertex u, where the influence decreases as the distance between v and u increases. More formally, δ is a decay factor (a constant between 0 and 1).

The accessibility index is a measure of the ease with which a vertex can access other vertices in the graph, considering the number of distinct paths to reach other vertices within a certain distance.

$$A(v,h) = \sum_{\tilde{\xi}=1}^{h} \frac{1}{\tilde{\xi}} \sum_{u\in V(G)} P^{\tilde{\xi}}(v,u),$$

where $P^{\tilde{\xi}}(v,u)$ is the number of distinct paths of length $\tilde{\xi}$ from v to u, and h is a horizon limit.

The Shimbel index, also known as the Shimbel distance or sometimes referred to as closeness centrality in certain contexts, was defined by Shimbel in his revolutionary work on communication networks [46]. The original reference to this concept can be found in Shimbel's 1953 paper.

$$C(v) = \sum_{u \in V(G)} d(v,u).$$

For notations, see Table 1.

Table 1. Summary of variables and terms.

Symbol/Term	Description
$G = (V, E)$	A simple, connected graph G with a vertex set V and edge set E
$d(u,v)$	Distance between vertices u and v in the graph G
$e = uv$	An edge connecting vertices u and v
$\theta_u(e)$	Number of vertices closer to u than v for edge $e = uv$
$\widetilde{C_v}$	Contribution of vertex v in the WA formula, normalized by distance
γ	Euler–Mascheroni constant, appearing in asymptotic expansions
$\mathcal{O}(\cdot)$	Big-O notation for higher-order terms in asymptotic expansions
$WA(G)$	Weighted asymmetry index of graph G
π	Number of vertices in the graph G
P_π	A path graph with π vertices
S_π	A star graph with π vertices
W_π	A wheel graph with π vertices
T_π	A tree of π vertices
$K_{\omega,\pi}$	A complete bipartite graph
$K_{\pi,\omega,\varphi}$	A complete tripartite graph

4. Results

In this section, we first define the weighted asymmetry index and then present the extremal graphs along with the exact results related to the weighted asymmetry index.

4.1. Weighted Asymmetry Index WA(G)

The weighted asymmetry index (WA) of a simple connected graph G is defined as

$$WA(G) = \sum_{e=uv \in E} \left| \sum_{w \in V} \theta_u(e) \cdot \left(\frac{1}{d(u,w)+1} \right) - \sum_{w \in V} \theta_v(e) \cdot \left(\frac{1}{d(v,w)+1} \right) \right|. \quad (1)$$

The term $\frac{1}{d(u,w)+1}$ is used to ensure a finite contribution to the index even when $d(u,w)$ is large or when $w = u$.

The index $WA(G)$ measures the aggregate difference between two sums for each edge $e = uv$, where each sum is over all vertices w in the graph. These sums weight the vertices w by their inverse distance (plus one) to u and v, respectively. Essentially, $WA(G)$ reflects how much more "influence" or "reach" vertex u has compared to v, aggregated over all vertices w, with distances appropriately normalized.

This index generalizes the idea of peripheral versus central influence in a graph, similarly to those indices, which measures peripherality by counting vertices closer to one end of an edge than the other. However, the WA index also accounts for the relative distances of all vertices, not just those on one side of an edge. Since the index depends

on distances in a non-linear way (through the reciprocal function), it is sensitive to the structure of the graph, particularly to how vertices are distributed relative to each edge.

This new index opens interesting avenues for further exploration, particularly in its mathematical properties and potential applications in various fields.

Example 1. *The path graph P_5 has 5 vertices arranged linearly, and can be represented as*

$$P_5 = (v_1 - v_2 - v_3 - v_4 - v_5).$$

- *Vertices:* $V(P_5) = \{v_1, v_2, v_3, v_4, v_5\}$.
- *Edges:* $E(P_5) = \{(v_1v_2), (v_2v_3), (v_3v_4), (v_4v_5)\}$.

We need to compute the weighted asymmetry index by going through each edge in P_5, calculating the sums for each vertex on both sides of each edge.

For edge $e = v_1v_2$:
$\theta_{v_1}(v_1v_2)$: All vertices closer to v_1 than to v_2 are v_1 itself. So, $\theta_{v_1}(v_1v_2) = 1$.
$\theta_{v_2}(v_1v_2)$: All vertices closer to v_2 than to v_1 are v_2, v_3, v_4, v_5. So, $\theta_{v_2}(v_1v_2) = 4$.
Distances from v_1:

$$\sum_{w \in V} \left(\frac{1}{d(v_1, w) + 1} \right) = \frac{1}{1} + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \frac{1}{5} = 1 + 0.5 + 0.333 + 0.25 + 0.2 = 2.283.$$

Distances from v_2:

$$\sum_{w \in V} \left(\frac{1}{d(v_2, w) + 1} \right) = \frac{1}{2} + \frac{1}{1} + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} = 0.5 + 1 + 0.5 + 0.333 + 0.25 = 2.583.$$

Contribution of edge v_1v_2:

$$\textit{Contribution} = |1 \cdot 2.283 - 4 \cdot 2.583| = |2.283 - 10.332| = 8.049.$$

Similar calculations can be performed for all other edges:
Distances from v_3:

$$\sum_{w \in V} \left(\frac{1}{d(v_3, w) + 1} \right) = \frac{1}{3} + \frac{1}{2} + \frac{1}{1} + \frac{1}{2} + \frac{1}{3} = 0.333 + 0.5 + 1 + 0.5 + 0.333 = 2.666.$$

Contribution of edge v_2v_3:

$$\textit{Contribution} = |2 \cdot 2.583 - 3 \cdot 2.666| = |5.166 - 7.998| = 2.832.$$

Distances from v_4:

$$\sum_{w \in V} \left(\frac{1}{d(v_4, w) + 1} \right) = \frac{1}{4} + \frac{1}{3} + \frac{1}{2} + \frac{1}{1} + \frac{1}{2} = 0.25 + 0.333 + 0.5 + 1 + 0.5 = 2.583.$$

Contribution of edge v_3v_4:

$$\textit{Contribution} = |3 \cdot 2.666 - 2 \cdot 2.583| = |7.998 - 5.166| = 2.832.$$

Distances from v_5:

$$\sum_{w \in V} \left(\frac{1}{d(v_5, w) + 1} \right) = \frac{1}{5} + \frac{1}{4} + \frac{1}{3} + \frac{1}{2} + \frac{1}{1} = 0.2 + 0.25 + 0.333 + 0.5 + 1 = 2.283.$$

Contribution of edge v_4v_5:

$$\textit{Contribution} = |4 \cdot 2.583 - 1 \cdot 2.283| = |10.332 - 2.283| = 8.049.$$

Finally, the contributions from all edges can be summed:

$$WA(P_5) = 8.049 + 2.832 + 2.832 + 8.049 = 21.762.$$

4.2. Extremal Values of Trees

Theorem 1. *Let P_π be a path graph of π vertices. Then,*

$$WA(P_\pi) = \sum_{\ddot{\vartheta}=1}^{\pi-1} \left| \ddot{\vartheta} \cdot \ln\big((\pi - \ddot{\vartheta} + 1) \cdot \ddot{\vartheta}\big) - (\pi - \ddot{\vartheta}) \cdot \ln\big((\pi - \ddot{\vartheta}) \cdot (\ddot{\vartheta} + 1)\big) + 4\gamma\ddot{\vartheta} - 2\gamma\pi + \pi - 2\ddot{\vartheta} \right.$$
$$\left. + \frac{\ddot{\vartheta}}{2(\pi - \ddot{\vartheta} + 1)} - \frac{\pi - \ddot{\vartheta}}{2(\ddot{\vartheta} + 1)} - \frac{\ddot{\vartheta}}{12(\pi - \ddot{\vartheta} + 1)^2} - \frac{1}{12\ddot{\vartheta}} + \frac{1}{12(\pi - \ddot{\vartheta})} + \frac{\pi - \ddot{\vartheta}}{12(\ddot{\vartheta} + 1)^2} + \mathcal{O}\left(\frac{1}{\ddot{\vartheta}^3}\right) \right|.$$

Here, γ is the Euler–Mascheroni constant, $\ddot{\vartheta}$ represents the index of a vertex, where $\ddot{\vartheta} \in \{1, 2, \ldots, \pi - 1\}$, and $\mathcal{O}\left(\frac{1}{\ddot{\vartheta}^3}\right)$ denotes the higher-order terms.

Proof. To compute the weighted asymmetry index $WA(P_\pi)$ for the path graph P_π with π vertices, we proceed as follows.

Each edge $e_{\ddot{\vartheta}} = v_{\ddot{\vartheta}} v_{\ddot{\vartheta}+1}$ in the path graph has two vertices: $v_{\ddot{\vartheta}}$ and $v_{\ddot{\vartheta}+1}$. The number of vertices closer to $v_{\ddot{\vartheta}}$ than $v_{\ddot{\vartheta}+1}$ is $\theta_{v_{\ddot{\vartheta}}}(e_{\ddot{\vartheta}}) = \ddot{\vartheta}$, while the number of vertices closer to $v_{\ddot{\vartheta}+1}$ is $\theta_{v_{\ddot{\vartheta}+1}}(e_{\ddot{\vartheta}}) = \pi - \ddot{\vartheta}$. This is because the path structure allows us to count the vertices on either side of $v_{\ddot{\vartheta}}$ and $v_{\ddot{\vartheta}+1}$.

The next step is to compute the weighted sums of distances for both vertices $v_{\ddot{\vartheta}}$ and $v_{\ddot{\vartheta}+1}$. These sums account for how each vertex in the graph influences the weighted asymmetry index based on its distance.

The weighted sum of distances for vertex $v_{\ddot{\vartheta}}$ is

$$\widetilde{C}_{v_{\ddot{\vartheta}}} = \sum_{w \in V} \frac{1}{d(v_{\ddot{\vartheta}}, w) + 1} = \sum_{\tilde{\xi}=0}^{\ddot{\vartheta}-1} \frac{1}{\tilde{\xi} + 1} + \sum_{\tilde{\xi}=1}^{\pi-\ddot{\vartheta}} \frac{1}{\tilde{\xi} + 1},$$

which captures the sum of reciprocal distances between $v_{\ddot{\vartheta}}$ and all other vertices.

Similarly, the weighted sum of distances for vertex $v_{\ddot{\vartheta}+1}$ is

$$\widetilde{C}_{v_{\ddot{\vartheta}+1}} = \sum_{w \in V} \frac{1}{d(v_{\ddot{\vartheta}+1}, w) + 1} = \sum_{\tilde{\xi}=1}^{\ddot{\vartheta}} \frac{1}{\tilde{\xi} + 1} + \sum_{\tilde{\xi}=0}^{\pi-\ddot{\vartheta}-1} \frac{1}{\tilde{\xi} + 1}.$$

These sums reflect the contribution from all vertices in P_π, calculated based on their distances to $v_{\ddot{\vartheta}}$ and $v_{\ddot{\vartheta}+1}$.

Now, for each edge $e_{\ddot{\vartheta}} = v_{\ddot{\vartheta}} v_{\ddot{\vartheta}+1}$, we compute the absolute difference between the weighted sums:

$$\left| \sum_{w \in V} \frac{\ddot{\vartheta}}{d(v_{\ddot{\vartheta}}, w) + 1} - \sum_{w \in V} \frac{\pi - \ddot{\vartheta}}{d(v_{\ddot{\vartheta}+1}, w) + 1} \right|.$$

The weighted asymmetry index $WA(P_\pi)$ is the sum of these absolute differences over all edges in the path graph:

$$WA(P_\pi) = \sum_{\ddot{\vartheta}=1}^{\pi-1} \left| \sum_{w \in V} \frac{\ddot{\vartheta}}{d(v_{\ddot{\vartheta}}, w) + 1} - \sum_{w \in V} \frac{\pi - \ddot{\vartheta}}{d(v_{\ddot{\vartheta}+1}, w) + 1} \right|.$$

Using the harmonic numbers $H_{\tilde{\xi}} = \sum_{\varsigma=1}^{\tilde{\xi}} \frac{1}{\varsigma}$, the index $WA(P_\pi)$ can be expressed as

$$WA(P_\pi) = \sum_{\ddot{\vartheta}=1}^{\pi-1} \left| \ddot{\vartheta} \cdot \left(H_{\pi-\ddot{\vartheta}+1} + H_{\ddot{\vartheta}} - 1\right) - (\pi - \ddot{\vartheta}) \cdot \left(H_{\pi-\ddot{\vartheta}} + H_{\ddot{\vartheta}+1} - 1\right) \right|.$$

$H_\pi \approx \ln(\pi) + \gamma + \frac{1}{2\pi} - \frac{1}{12\pi^2} + \mathcal{O}\left(\frac{1}{\pi^4}\right)$, and the weighted sums can be simplified further. Substituting the approximations for $H_{\pi-\ddot{\vartheta}+1}$, $H_{\ddot{\vartheta}}$, $H_{\pi-\ddot{\vartheta}}$, and $H_{\ddot{\vartheta}+1}$ into the formula for $WA(P_\pi)$, we obtain the following:

$$WA(P_\pi) = \sum_{\ddot{\vartheta}=1}^{\pi-1} \Bigg| \ddot{\vartheta} \cdot \Bigg(\ln(\pi - \ddot{\vartheta} + 1) + \ln(\ddot{\vartheta}) + 2\gamma + \frac{1}{2(\pi - \ddot{\vartheta} + 1)} + \frac{1}{2\ddot{\vartheta}} - \frac{1}{12(\pi - \ddot{\vartheta} + 1)^2} - \frac{1}{12\ddot{\vartheta}^2} + \mathcal{O}\left(\frac{1}{(\pi - \ddot{\vartheta} + 1)^4}\right) + \mathcal{O}\left(\frac{1}{\ddot{\vartheta}^4}\right) - 1 \Bigg) - (\pi - \ddot{\vartheta}) \cdot \big(\ln(\pi - \ddot{\vartheta}) + \ln(\ddot{\vartheta} + 1) + 2\gamma + \frac{1}{2(\pi - \ddot{\vartheta})} + \frac{1}{2(\ddot{\vartheta} + 1)} - \frac{1}{12(\pi - \ddot{\vartheta})^2} - \frac{1}{12(\ddot{\vartheta} + 1)^2} + \mathcal{O}\left(\frac{1}{(\pi - \ddot{\vartheta})^4}\right) + \mathcal{O}\left(\frac{1}{(\ddot{\vartheta} + 1)^4}\right) - 1\Big) \Bigg|$$

$$WA(P_\pi) = \sum_{\ddot{\vartheta}=1}^{\pi-1} \Bigg| \ddot{\vartheta} \cdot \ln\big((\pi - \ddot{\vartheta} + 1) \cdot \ddot{\vartheta}\big) - (\pi - \ddot{\vartheta}) \cdot \ln\big((\pi - \ddot{\vartheta}) \cdot (\ddot{\vartheta} + 1)\big) + 2\gamma(2\ddot{\vartheta} - \pi) + (\pi - 2\ddot{\vartheta}) + \frac{\ddot{\vartheta}}{2(\pi - \ddot{\vartheta} + 1)} + \frac{\ddot{\vartheta}}{2\ddot{\vartheta}} - \frac{\pi - \ddot{\vartheta}}{2(\pi - \ddot{\vartheta})} - \frac{\pi - \ddot{\vartheta}}{2(\ddot{\vartheta} + 1)} - \frac{\ddot{\vartheta}}{12(\pi - \ddot{\vartheta} + 1)^2} - \frac{\ddot{\vartheta}}{12\ddot{\vartheta}^2} + \frac{\pi - \ddot{\vartheta}}{12(\pi - \ddot{\vartheta})^2} + \frac{\pi - \ddot{\vartheta}}{12(\ddot{\vartheta} + 1)^2} + \mathcal{O}\left(\frac{1}{\ddot{\vartheta}^3}\right) \Bigg|.$$

$$WA(P_\pi) = \sum_{\ddot{\vartheta}=1}^{\pi-1} \Bigg| \ddot{\vartheta} \cdot \ln\big((\pi - \ddot{\vartheta} + 1) \cdot \ddot{\vartheta}\big) - (\pi - \ddot{\vartheta}) \cdot \ln\big((\pi - \ddot{\vartheta}) \cdot (\ddot{\vartheta} + 1)\big) + 4\gamma\ddot{\vartheta} - 2\gamma\pi + \pi - 2\ddot{\vartheta} + \frac{\ddot{\vartheta}}{2(\pi - \ddot{\vartheta} + 1)} - \frac{\pi - \ddot{\vartheta}}{2(\ddot{\vartheta} + 1)} - \frac{\ddot{\vartheta}}{12(\pi - \ddot{\vartheta} + 1)^2} - \frac{1}{12\ddot{\vartheta}} + \frac{1}{12(\pi - \ddot{\vartheta})} + \frac{\pi - \ddot{\vartheta}}{12(\ddot{\vartheta} + 1)^2} + \mathcal{O}\left(\frac{1}{\ddot{\vartheta}^3}\right). \Bigg|$$

□

Since the vertices of the path graphs are arranged in a linear sequence, the value of the WA index of path graphs on n vertices is usually small because the path graph tends to be highly symmetric. It may be said that the central vertices can be considered equidistant from other vertices, but the end vertices bring some imbalance. A small value of the WA index in a path graph demonstrates that the vertices are spread symmetrically so that no vertex dominates the structure in terms of connectivity or distance. This means that the flow of information or transport is moderately efficient since the longest paths can exist only between the end vertices. Still, symmetry reduces the probability that bottlenecks or weak points exist in the network.

Theorem 2. *Let S_π be a star graph with π vertices. Then,*

$$WA(S_\pi) = \frac{1}{2}\pi^3 - \pi - \frac{5}{6}\pi^2 + \frac{4}{3}.$$

Proof. A star graph S_π consists of one central vertex v_c and $\pi - 1$ pendant vertices $v_1, v_2, \ldots, v_{\pi-1}$. Each pendant vertex is connected only to the central vertex v_c, so there are $\pi - 1$ edges in the graph.

To find the $WA(S_\pi)$, first we calculate $\theta_{v_{c(e)}}$ and $\theta_{v_{\ddot{\vartheta}}}(e)$ for each edge $e = v_c v_{\ddot{\vartheta}}$ in the star graph S_π.

All vertices except $v_{\ddot{\vartheta}}$ are closer to v_c because v_c is directly connected to all other vertices. Therefore,

$$\theta_{v_c}(e) = \pi - 1.$$

$$\theta_{v_{\ddot{\vartheta}}}(e) = 1.$$

Now,

$$\widetilde{C_{v_c}} = \sum_{w \in V(S_\pi)} \frac{1}{d(v_c, w) + 1} = \frac{1}{1} + (\pi - 1) \cdot \frac{1}{2} = 1 + \frac{\pi - 1}{2},$$

and

$$\widetilde{C_{v_{\ddot{\vartheta}}}} = \frac{1}{1} + \frac{1}{2} + (\pi - 2) \cdot \frac{1}{3} = 1 + \frac{1}{2} + \frac{\pi - 2}{3}.$$

The total index $WA(S_\pi)$ for the star graph is the sum of contributions from all edges $v_c v_{\ddot{\vartheta}}$ for $1 \leq \ddot{\vartheta} \leq \pi - 1$:

$$WA(S_\pi) = \sum_{\ddot{\vartheta}=1}^{\pi-1} \left| (\pi - 1) \cdot \left(1 + \frac{\pi - 1}{2}\right) - 1 \cdot \left(1 + \frac{1}{2} + \frac{\pi - 2}{3}\right) \right|.$$

$$WA(S_\pi) = (\pi - 1) \times \left| (\pi - 1) \cdot \left(1 + \frac{\pi - 1}{2}\right) - 1 \cdot \left(1 + \frac{1}{2} + \frac{\pi - 2}{3}\right) \right|.$$

After simplifying, we obtain

$$WA(S_\pi) = \frac{1}{2}\pi^3 - \pi - \frac{5}{6}\pi^2 + \frac{4}{3}.$$

□

A generalized star graph $S_{\pi,\varpi}$ is a graph consisting of π paths, each of length ϖ, denoted as P_ϖ. The paths are arranged such that they all have a common central vertex v_c. The central vertex v_c is connected to the first vertex $v_{\ddot{\vartheta},1}$ of each path P_ϖ for $1 \leq \ddot{\vartheta} \leq \pi$. For each path P_ϖ, the vertices are connected sequentially, meaning that $v_{\ddot{\vartheta},\varsigma}$ is connected to $v_{\ddot{\vartheta},\varsigma+1}$ for $1 \leq \varsigma \leq \varpi - 1$.

Theorem 3. *Let $S_{\pi,\varpi}$ be a generalized star graph. Then,*

$$WA(S_{\pi,\varpi}) = (\pi\varpi - \pi)(\ln(\varsigma) + \ln(\varpi - \varsigma + 1) + \ln(\varsigma + \varpi + 1) - (\pi - 1)\ln(\varsigma + 1) + 2\gamma + \frac{1}{\varsigma + 1} + \mathcal{O}\left(\frac{1}{\varsigma^2}\right)\Big)|\pi\varpi - 2\varpi + 2\varsigma + 1| + \pi\Big|(\pi\varpi - \varpi + 1)\Big(\pi\ln(\varpi + 1) + \pi\gamma + \frac{\pi}{2(\varpi + 1)} - \frac{\pi}{12(\varpi + 1)^2} + \mathcal{O}\Big(\frac{1}{(\varpi + 1)^3}\Big)\Big) - \varpi \cdot \Big(\ln(\varpi + 1) + \gamma + \frac{1}{2} + \frac{\pi - 1}{\varpi + 1} + \frac{\pi - 1}{\varpi + 2} + \frac{1}{2(\varpi + 1)} - \frac{1}{12(\varpi + 1)^2} + \mathcal{O}\Big(\frac{1}{\varpi^3}\Big)\Big)\Big|.$$

Proof. To compute the weighted asymmetry index for the generalized star graph $S_{\pi,\varpi}$, we begin by calculating the centrality measures $\widetilde{C_v}$ and the values of $\theta_v(e)$ for different vertices in the graph.

Let us first consider the distances to other vertices on the same path $P_{\ddot{\vartheta}}$ as $v_{\ddot{\vartheta},\varsigma}$. $d(v_{\ddot{\vartheta},\varsigma}, v_{\ddot{\vartheta},\tilde{\xi}}) = |\varsigma - \tilde{\xi}|$, where $\tilde{\xi}$ is any other index in the same path $P_{\ddot{\vartheta}}$, where $1 \leq \ddot{\vartheta} \leq \pi$ and $1 \leq \varsigma \leq \varpi$. Thus, the contribution from all vertices on the same path is

$$\sum_{\tilde{\xi}=1}^{\varpi} \frac{1}{|\varsigma - \tilde{\xi}| + 1}.$$

For paths $P_{\tilde{\xi}}$, where $\tilde{\xi} \neq \ddot{\vartheta}$, i.e., all other paths are attached to v_c, any vertex $v_{\tilde{\xi},p}$ on a different path $P_{\tilde{\xi}}$ is at distance $\varsigma + p$ from $v_{\ddot{\vartheta},\varsigma}$ (this is the sum of the distance from $v_{\ddot{\vartheta},\varsigma}$ to v_c, which is ς, plus the distance from v_c to $v_{\tilde{\xi},p}$, which is p). The contribution from all vertices on these other paths is

$$\sum_{\tilde{\xi} \neq \ddot{\vartheta}} \sum_{p=1}^{\varpi} \frac{1}{\varsigma + p + 1}.$$

The distance from $v_{\ddot{\vartheta},\varsigma}$ to the central vertex v_c is $d(v_{\ddot{\vartheta},\varsigma}, v_c) = \varsigma$ (since there are ς edges between $v_{\ddot{\vartheta},\varsigma}$ and v_c). The contribution from the central vertex v_c is

$$\frac{1}{\varsigma+1}.$$

Combining all these contributions, we obtain

$$\widetilde{C_{v_{\ddot{\vartheta},\varsigma}}} = \sum_{\tilde{\xi}=1}^{\varpi} \frac{1}{|\varsigma - \tilde{\xi}| + 1} + \frac{1}{\varsigma+1} + \sum_{\tilde{\xi}\neq\ddot{\vartheta}} \sum_{p=1}^{\varpi} \frac{1}{\varsigma+p+1}.$$

The distance from v_c to itself is $d(v_c, v_c) = 0$, so the contribution from v_c is $\frac{1}{0+1} = 1$. Each $v_{\ddot{\vartheta},1}$ is directly connected to v_c, so the distance $d(v_c, v_{\ddot{\vartheta},1}) = 1$. The contribution from all such vertices is

$$\pi \times \frac{1}{1+1} = \pi \times \frac{1}{2}.$$

Now, for each path $\ddot{\vartheta}$, the vertices $v_{\ddot{\vartheta},2}, v_{\ddot{\vartheta},3}, \ldots, v_{\ddot{\vartheta},\varpi}$ are progressively further from v_c. The distance from v_c to $v_{\ddot{\vartheta},\varsigma}$ is $d(v_c, v_{\ddot{\vartheta},\varsigma}) = \varsigma$. Thus, the contribution from these vertices is

$$\sum_{\ddot{\vartheta}=1}^{\pi} \sum_{\varsigma=2}^{\varpi} \frac{1}{\varsigma+1}.$$

Since each path contributes the same, this simplifies to

$$\pi \sum_{\tilde{\xi}=2}^{\varpi} \frac{1}{\tilde{\xi}+1}.$$

Thus, combining all these contributions, we have

$$\widetilde{C_{v_c}} = 1 + \pi \sum_{\tilde{\xi}=1}^{\varpi} \frac{1}{\tilde{\xi}+1}.$$

For each edge $e_{\ddot{\vartheta}} = v_c v_{\ddot{\vartheta},1}$ in the graph, the number of vertices closer to v_c than $v_{\ddot{\vartheta},1}$ is $\theta_{v_c}(e) = \pi\varpi - \varpi + 1$, and the number of vertices closer to $v_{\ddot{\vartheta},1}$ than v_c is $\theta_{v_{\ddot{\vartheta},1}}(e_{\ddot{\vartheta}}) = \varpi$.

For each edge $e_{\ddot{\vartheta}} = v_{\ddot{\vartheta},\varsigma} v_{\ddot{\vartheta},\varsigma+1}$ in the graph, the number of vertices closer to $v_{\ddot{\vartheta},\varsigma}$ is

$$\theta_{v_{\ddot{\vartheta},\varsigma}}(e) = \pi\varpi - \varpi + \varsigma + 1,$$

and for the adjacent vertex $v_{\ddot{\vartheta},\varsigma+1}$ it is

$$\theta_{v_{\ddot{\vartheta},\varsigma+1}}(e) = \varpi - \varsigma.$$

We now insert these centrality measures and vertex contribution values into the formula for the weighted asymmetry index. The formula is given by

$$WA(S_{\pi,\varpi}) = \sum_{e\in E(S_{\pi,\varpi})} |\theta_u(e) C_u - \theta_v(e) C_v|.$$

Substituting the specific values for $\theta_u(e)$ and $\widetilde{C_u}$, we obtain

$$WA(S_{\pi,\varpi}) = (\varpi-1)\pi\Bigg|(\pi\varpi-\varpi+\varsigma+1)\cdot\left(1+\sum_{\tilde{\xi}=1}^{\varpi}\frac{1}{|\varsigma-\tilde{\xi}|+1}+\frac{1}{\varsigma+1}+(\pi-1)\sum_{p=1}^{\varpi}\frac{1}{\varsigma+p+1}\right)$$
$$-(\varpi-\varsigma)\left(1+\sum_{\tilde{\xi}=1}^{\varpi}\frac{1}{|\varsigma-\tilde{\xi}|+1}+\frac{1}{\varsigma+1}+(\pi-1)\sum_{p=1}^{\varpi}\frac{1}{\varsigma+p+1}\right)\Bigg|+\pi\Bigg|(\pi\varpi-\varpi+1)\left(1+\pi\sum_{\tilde{\xi}=1}^{\varpi}\frac{1}{\tilde{\xi}+1}\right) \quad (2)$$
$$-\varpi\left(2+\sum_{\tilde{\xi}=1}^{\varpi-1}\frac{1}{\tilde{\xi}+2}+\frac{\pi-1}{\varpi+1}+\frac{\pi-1}{\varpi+2}\right)\Bigg|.$$

We now simplify the sum $\sum_{\tilde{\xi}=1}^{\varpi}\frac{1}{|\varsigma-\tilde{\xi}|+1}$, separating it into three cases.

For $\tilde{\xi}=\varsigma$:

$$\frac{1}{|\varsigma-\varsigma|+1}=1.$$

For $\tilde{\xi}\neq\varsigma$:

When $\tilde{\xi}<\varsigma$, we introduce the substitution $p=\varsigma-\tilde{\xi}$, and the sum becomes $\sum_{p=1}^{\varsigma-1}\frac{1}{p+1}$.

When $\tilde{\xi}>\varsigma$, we substitute $p=\tilde{\xi}-\varsigma$, giving $\sum_{p=1}^{\varpi-\varsigma}\frac{1}{p+1}$.

Thus, we combine the two parts:

$$\sum_{\tilde{\xi}=1}^{\varpi}\frac{1}{|\varsigma-\tilde{\xi}|+1}=H_{\varsigma}+H_{\varpi-\varsigma+1}-1.$$

where H_{π} is the π-th harmonic number.

For large ς and $\varpi-\varsigma+1$, harmonic numbers can be approximated as

$$H_{\varsigma}\approx\ln(\varsigma)+\gamma+\frac{1}{2\varsigma}-\frac{1}{12\varsigma^2}+\mathcal{O}\left(\frac{1}{\varsigma^3}\right).$$

$$H_{\varpi-\varsigma+1}\approx\ln(\varpi-\varsigma+1)+\gamma+\frac{1}{2(\varpi-\varsigma+1)}-\frac{1}{12(\varpi-\varsigma+1)^2}+\mathcal{O}\left(\frac{1}{(\varpi-\varsigma+1)^3}\right).$$

Similarly,

$$\sum_{p=1}^{\varpi}\frac{1}{\varsigma+p+1}\approx\ln(\varsigma+\varpi+1)-\ln(\varsigma+1)+\mathcal{O}\left(\frac{1}{\varsigma^2}\right).$$

$$\sum_{\tilde{\xi}=1}^{\varpi}\frac{1}{\tilde{\xi}+1}\approx\ln(\varpi+1)+\gamma-1+\mathcal{O}\left(\frac{1}{\varpi^3}\right).$$

Inserting these harmonic approximations into Equation (2), we obtain

$$WA(S_{\pi,\varpi})=(\pi\varpi-\pi)(\ln(\varsigma)+\ln(\varpi-\varsigma+1)+\ln(\varsigma+\varpi+1)-(\pi-1)\ln(\varsigma+1)+$$
$$2\gamma+\frac{1}{\varsigma+1}+\mathcal{O}\left(\frac{1}{\varsigma^2}\right)\Bigg)|\pi\varpi-2\varpi+2\varsigma+1|+\pi\Bigg|(\pi\varpi-\varpi+1)\Bigg(\pi\ln(\varpi+1)+\pi\gamma+\frac{\pi}{2(\varpi+1)}$$
$$-\frac{\pi}{12(\varpi+1)^2}+\mathcal{O}\left(\frac{1}{(\varpi+1)^3}\right)\Bigg)-\varpi\cdot\left(\ln(\varpi+1)+\gamma+\frac{1}{2}+\frac{\pi-1}{\varpi+1}+\frac{\pi-1}{\varpi+2}+\frac{1}{2(\varpi+1)}-\right.$$
$$\left.\frac{1}{12(\varpi+1)^2}+\mathcal{O}\left(\frac{1}{\varpi^3}\right)\right)\Bigg|.$$

□

Conjecture 1. *Consider T_π to be a tree of π vertices. Then,*

$$WA(P_\pi) \leq WA(T_\pi) \leq WA(S_\pi).$$

4.3. Weighted Asymmetry Index for Different Families of Graphs

Theorem 4. *Let $K_{\varpi,\pi}$ be a complete bipartite graph with vertex partition sets U and V of cardinality ϖ and π, ($\varpi > \pi$), respectively. Then the weighted asymmetry index of $K_{\varpi,\pi}$ is given by*

$$WA(K_{\varpi,\pi}) = \frac{1}{3}(\varpi^3\pi - \pi^3\varpi + 2\varpi^2\pi - 2\pi^2\varpi).$$

Proof. Consider the complete bipartite graph $K_{\varpi,\pi}$ with vertex partition U and V, where $|U| = \varpi$ and $|V| = \pi$. An edge $e = u_{\ddot{\vartheta}}v_{\varsigma}$ connects a vertex $u_{\ddot{\vartheta}} \in U$ and a vertex $v_{\varsigma} \in V$. We need to calculate the distances $d(u_{\ddot{\vartheta}}, w)$ and $d(v_{\varsigma}, w)$ for all vertices $w \in V(K_{\varpi,\pi})$, and then compute the contributions to the weighted asymmetry index from both $u_{\ddot{\vartheta}}$ and v_{ς}.

For a vertex $w \in U$, $d(u_{\ddot{\vartheta}}, w) = 0$ if $w = u_{\ddot{\vartheta}}$, $d(u_{\ddot{\vartheta}}, w) = 2$ if $w \neq u_{\ddot{\vartheta}}$ (since vertices in U are connected to each other through vertices in V), and $d(v_{\varsigma}, w) = 1$ for all $w \in U$. Thus, for a vertex $u_{\ddot{\vartheta}} \in U$, the total weighted centrality is

$$\widetilde{C_{u_{\ddot{\vartheta}}}} = 1 + \frac{\pi}{2} + (\varpi - 1) \times \frac{1}{3}.$$

Similarly, for a vertex $v_{\ddot{\vartheta}} \in V$,

$$\widetilde{C_{v_{\ddot{\vartheta}}}} = 1 + \frac{\varpi}{2} + (\pi - 1) \times \frac{1}{3}.$$

The total contribution of the edge $e = u_{\ddot{\vartheta}}v_{\varsigma}$ to the weighted asymmetry index is given by the absolute difference of the contributions from $u_{\ddot{\vartheta}}$ and v_{ς}:

$$\left|\varpi\left(1 + \frac{\varpi - 1}{3} + \frac{\pi}{2}\right) - \pi\left(1 + \frac{\pi - 1}{3} + \frac{\varpi}{2}\right)\right|.$$

Simplifying the expression inside the absolute value,

$$\left|\varpi\left(1 + \frac{\varpi - 1}{3} + \frac{\pi}{2}\right) - \pi\left(1 + \frac{\pi - 1}{3} + \frac{\varpi}{2}\right)\right| = \frac{1}{3}\left|\varpi^2 - \pi^2 + 2\varpi - 2\pi\right|.$$

Multiplying by the total number of edges $\pi\varpi$ in the complete bipartite graph $K_{\varpi,\pi}$, we obtain

$$WA(K_{\varpi,\pi}) = \frac{1}{3}\pi\varpi\left|\varpi^2 - \pi^2 + 2\varpi - 2\pi\right|.$$

Thus, the weighted asymmetry index for the complete bipartite graph $K_{\varpi,\pi}$ is

$$WA(K_{\varpi,\pi}) = \frac{1}{3}(\varpi^3\pi - \pi^3\varpi + 2\varpi^2\pi - 2\pi^2\varpi)$$

Since, we assume $\varpi > \pi$, we can omit the absolute value sign, leading to the simplified expression. □

Theorem 5. *Let W_π be a wheel graph with π vertices. Then,*

$$WA(W_\pi) = \frac{1}{2}\pi^3 - \frac{11}{6}\pi^2 - \frac{4}{3}\pi + \frac{8}{3}.$$

Proof. Let W_π be a wheel graph with π vertices, where the central vertex v_c is connected to the $\pi - 1$ vertices that form a cycle. We proceed by calculating the centrality measures for the central vertex v_c and the peripheral vertices $v_{\ddot{\vartheta}}$, as well as their contributions to the weighted asymmetry index.

The central vertex v_c is connected to all $\pi - 1$ peripheral vertices. Its centrality measure is given by:

$$\widetilde{C_{v_c}} = 1 + \frac{\pi - 1}{2}.$$

Each peripheral vertex $v_{\ddot{\vartheta}}$ is connected to the central vertex v_c and its two adjacent vertices in the cycle. The centrality measure for each $v_{\ddot{\vartheta}}$ is

$$\widetilde{C_{v_{\ddot{\vartheta}}}} = 1 + \frac{3}{2} + \frac{\pi - 4}{3}.$$

For each edge $e = v_c v_{\ddot{\vartheta}}$ connecting the central vertex v_c to a peripheral vertex $v_{\ddot{\vartheta}}$, the number of vertices closer to v_c are $\theta_{v_c} = \pi - 3$, and the number of vertices closer to $v_{\ddot{\vartheta}}$ is $\theta_{v_{\ddot{\vartheta}}} = 1$.

Thus, the contribution of each edge $e = v_c v_{\ddot{\vartheta}}$ to the weighted asymmetry index is

$$\left|(\pi - 3) \cdot \widetilde{C_{v_c}} - \widetilde{C_{v_{\ddot{\vartheta}}}}\right|.$$

In terms of the contribution from cycle edges $e = v_{\ddot{\vartheta}} v_{\ddot{\vartheta}+1}$, for each edge $e = v_{\ddot{\vartheta}} v_{\ddot{\vartheta}+1}$ connecting two adjacent peripheral vertices in the cycle, both vertices $v_{\ddot{\vartheta}}$ and $v_{\ddot{\vartheta}+1}$ have two neighbors in the cycle. The number of vertices closer to both $v_{\ddot{\vartheta}}$ and $v_{\ddot{\vartheta}+1}$ is $\theta_{v_{\ddot{\vartheta}}} = \theta_{v_{\ddot{\vartheta}+1}} = 2$. Thus, the contribution of each cycle edge $e = v_{\ddot{\vartheta}} v_{\ddot{\vartheta}+1}$ is

$$\left|2 \cdot \widetilde{C_{v_{\ddot{\vartheta}}}} - 2 \cdot \widetilde{C_{v_{\ddot{\vartheta}+1}}}\right| = 0.$$

The total weighted asymmetry index $WA(W_\pi)$ for the wheel graph is the sum of the contributions from the $\pi - 1$ central edges. The cycle edges contribute nothing, so the final expression is

$$WA(W_\pi) = \pi - 1 \cdot \left|(\pi - 3) \cdot \left(1 + \frac{\pi}{2}\right) - \left(2.5 + \frac{\pi - 4}{3}\right)\right|.$$

$$WA(W_\pi) = \frac{1}{2}\pi^3 - \frac{11}{6}\pi^2 - \frac{4}{3}\pi + \frac{8}{3}.$$

□

Theorem 6. *Let $K_{\pi,\varpi,\varphi}$ be a complete tripartite graph with vertex partition sets U, V, and W of cardinality π, ϖ, and φ, respectively. Then, the weighted asymmetry index of $K_{\pi,\varpi,\varphi}$ is*

$$WA(K_{\pi,\varpi,\varphi}) = \left|\frac{1}{2}\pi\varpi\varphi^3 + \frac{2}{3}\pi\varphi^2 - \frac{1}{2}\pi^3\varpi\varphi - \frac{2}{3}\pi^2\varphi\right| + \left|\frac{1}{2}\pi\varpi^3\varphi + \frac{2}{3}\pi\varpi^2 - \frac{1}{2}\pi^3\varpi\varphi - \frac{2}{3}\pi^2\varpi\right| + \left|\frac{1}{2}\pi\varpi^3\varphi + \frac{2}{3}\varpi^2\varphi - \frac{1}{2}\pi\varpi\varphi^3 - \frac{2}{3}\varpi\varphi^2\right|.$$

Proof. Consider the complete tripartite graph $K_{\pi,\varpi,\varphi}$ with vertex partition sets U, V, and W, where $|U| = \pi$, $|V| = \varpi$, and $|W| = \varphi$. The edges of $K_{\pi,\varpi,\varphi}$ connect vertices $u_{\ddot{\vartheta}} \in U$ with vertices $v_\varsigma \in V$, vertices $u_{\ddot{\vartheta}} \in U$ with vertices $w_{\tilde{\xi}} \in W$, and vertices $v_\varsigma \in V$ with vertices $w_{\tilde{\varsigma}} \in W$.

Now, we calculate the distances for all vertices $\alpha \in V(K_{\pi,\varpi,\varphi})$ and compute the contributions to the weighted asymmetry index from these distances. For each vertex in the partitions U, V, and W, the centrality measures $\widetilde{C}$ are as follows:

For a vertex $u_{\ddot{\vartheta}} \in U$:

$$\widetilde{C_{u_{\ddot{\vartheta}}}} = 1 + \frac{\varpi\varphi}{2} + (\pi - 1) \cdot \frac{1}{3}.$$

For a vertex $v_\varsigma \in V$:

$$\widetilde{C_{v_\varsigma}} = 1 + \frac{\pi\varphi}{2} + (\varpi - 1) \cdot \frac{1}{3}.$$

For a vertex $w_{\tilde{\xi}} \in W$:

$$\widetilde{C_{w_{\tilde{\xi}}}} = 1 + \frac{\pi\varpi}{2} + (\varphi - 1) \cdot \frac{1}{3}.$$

For each edge e_s in the graph, the number of vertices closer to each endpoint is as follows.

For an edge $e_s = u_{\ddot{\vartheta}} v_\varsigma$, the number of vertices closer to $u_{\ddot{\vartheta}}$ than v_ς is $\theta_{u_{\ddot{\vartheta}}}(e_s) = \varpi$, and the number of vertices closer to v_ς than $u_{\ddot{\vartheta}}$ is $\theta_{v_\varsigma}(e_s) = \pi$.

Similarly, for an edge $e_s = u_{\ddot{\vartheta}} w_{\tilde{\xi}}$, the number of vertices closer to $u_{\ddot{\vartheta}}$ than $w_{\tilde{\xi}}$ is $\theta_{u_{\ddot{\vartheta}}}(e_s) = \varphi$, and the number of vertices closer to $w_{\tilde{\xi}}$ than $u_{\ddot{\vartheta}}$ is $\theta_{w_{\tilde{\xi}}}(e_s) = \pi$.

Finally, for an edge $e_s = v_\varsigma w_{\tilde{\xi}}$, the number of vertices closer to v_ς than $w_{\tilde{\xi}}$ is $\theta_{v_\varsigma}(e_s) = \varphi$, and the number of vertices closer to $w_{\tilde{\xi}}$ than v_ς is $\theta_{w_{\tilde{\xi}}}(e_s) = \varpi$.

The total weighted asymmetry index $WA(K_{\pi,\varpi,\varphi})$ is the sum of contributions from all the edges in $K_{\pi,\varpi,\varphi}$. Each edge contributes according to the following formula:

$$WA(K_{\pi,\varpi,\varphi}) = \sum_{e_s \in E(K_{\pi,\varpi,\varphi})} \left| \theta_u(e_s) \cdot \widetilde{C_u} - \theta_v(e_s) \cdot \widetilde{C_v} \right|.$$

Substituting the computed values for $\theta_u(e_s)$, $\theta_v(e_s)$, $\widetilde{C_u}$, and $\widetilde{C_v}$, we obtain
Contribution from edges $u_{\ddot{\vartheta}} v_\varsigma$ (between U and V):

$$\pi\varpi \left| \varpi \left(1 + \frac{\varpi\varphi}{2} + (\pi - 1) \cdot \frac{1}{3} \right) - \pi \left(1 + \frac{\pi\varphi}{2} + (\varpi - 1) \cdot \frac{1}{3} \right) \right|.$$

Contribution from edges $u_{\ddot{\vartheta}} w_{\tilde{\xi}}$ (between U and W):

$$\pi\varphi \left| \varphi \left(1 + \frac{\varpi\varphi}{2} + (\pi - 1) \cdot \frac{1}{3} \right) - \pi \left(1 + \frac{\pi\varpi}{2} + (\varphi - 1) \cdot \frac{1}{3} \right) \right|.$$

Contribution from edges $v_\varsigma w_{\tilde{\xi}}$ (between V and W):

$$\varpi\varphi \left| \varpi \left(1 + \frac{\pi\varpi}{2} + (\varphi - 1) \cdot \frac{1}{3} \right) - \varphi \left(1 + \frac{\pi\varphi}{2} + (\varpi - 1) \cdot \frac{1}{3} \right) \right|.$$

Simplifying these contributions leads to the final expression for the weighted asymmetry index of $K_{\pi,\varpi,\varphi}$:

$$\begin{aligned} WA(K_{\pi,\varpi,\varphi}) = &\left| \frac{1}{2}\pi\varpi\varphi^3 + \frac{2}{3}\pi\varphi^2 - \frac{1}{2}\pi^3\varpi\varphi - \frac{2}{3}\pi^2\varphi \right| + \left| \frac{1}{2}\pi\varpi^3\varphi + \frac{2}{3}\pi\varpi^2 - \frac{1}{2}\pi^3\varpi\varphi - \frac{2}{3}\pi^2\varpi \right| \\ &+ \left| \frac{1}{2}\pi\varpi^3\varphi + \frac{2}{3}\varpi^2\varphi - \frac{1}{2}\pi\varpi\varphi^3 - \frac{2}{3}\varpi\varphi^2 \right|. \end{aligned}$$

□

4.4. Comparison of WA Index with Traditional Graph Indices

In Table 2, we compare WA to some other traditional graph indices, namely the Wiener index, Szeged index, and Mostar index, on three graph types: the path graph, the star graph, and the wheel graph. While the numerical trends for these various indices are approximately parallel to one another, the unusual information about structural imbalances contained in WA is not fully captured by the more traditional indices of asymmetric graph structures.

Table 2. Comparison of indices for selected graphs.

Graph	Wiener Index	Szeged Index	Mostar Index	WA Index
P_5	20	10	4	21.762
S_5	20	20	16	38
W_5	12	12	4	12.667

Path Graph P_5: Although this graph is relatively symmetric, the WA index detects slight imbalances due to the distances between the end vertices and the central vertices. The lower WA value reflects the moderate level of asymmetry present in this structure, as compared to the more pronounced asymmetry in the star and wheel graphs.

Star Graph S_5: The WA index reveals the significant asymmetry caused by the dominant central vertex, which is connected to all peripheral vertices. Traditional indices, such as the Wiener and Szeged indices, do not fully capture this centralization, as they primarily focus on aggregate distances. The higher WA value for the star graph highlights the sharp contrast in vertex distances from the hub, making the WA index more sensitive to centralized structures where one vertex is disproportionately important.

Wheel Graph W_5: The WA index once again identifies the asymmetry between the central hub and the peripheral cycle. While traditional indices provide similar values, they do not emphasize the asymmetry between the vertices in the cycle and the central hub as strongly. The WA index shows how the central vertex in the wheel graph influences the network's structure, a critical feature in systems where central nodes serve as critical communication points

By admitting the local asymmetries that are major contributors to the WA index, the structural imbalance in graphs has undergone deeper analysis with the WA index than with many other indices that detect trends in symmetry. The presence of a dominant vertex, like in the star and wheel graphs, is very significantly shown up by the disproportionate importance of that vertex when compared to traditional distance-based measures. The WA index in particular becomes very useful in network resilience analysis, in which it unequivocally points out critical vertices holding disproportionate influence. Also, in molecular graphs, the WA index provides a detailed view of the local asymmetry in bond lengths and vertex positions, which is essential for understanding molecular behavior. Unlike the Wiener or Szeged indices, which treat all vertex pairs similarly, the WA index captures these local structural differences, providing insight into molecular properties that affect chemical reactivity.

5. Applications

The weighted asymmetry index has important applications in wide areas where understanding the structural properties of graphs is necessary. Important areas where this index can be applied include the following.

5.1. Network Analysis

In communications networks, the weighted asymmetry index can be used to evaluate the efficiency and dependability of data exchange. Networks with a smaller asymmetry (smaller weighted asymmetry index) usually contain traffic distributed in a more uniform way, which is indicative of good load balancing and low latency. In social networks, the weighted asymmetry index can help identify asymmetries in relationships or communication flows. It indicates those key influencers, or nodes of power, with respect to spreading information.

5.2. Molecular Chemistry

In the study of molecular structures, the weighted asymmetry index makes it possible to visualize the symmetry and the distribution of atoms within a molecule. More relevantly, this would help in predicting better chemical properties and reactivity of the molecule. For

instance, molecules with high asymmetry may act in a different way chemically than more symmetric ones. The insight gained in drug design concerning the asymmetry of molecular structures is important to further predict how a drug will interact with a target protein. It could be used in optimizing weighted asymmetry indices for molecular structures with improved binding affinity and efficacy.

5.3. Computer Science

It can also be used in parallel processing to weight the asymmetry index assessing the load balancing amongst processors. If there is less asymmetry, that is, a lower weighted asymmetry index, there is better distribution and hence perhaps more efficient parallel processing. Therefore, the weighted asymmetry index can be used in the design of data structures, especially those that can easily be visualized as graphs like trees and heaps to study balance and optimize performance.

5.4. Polymer Science

An asymmetric index can weigh and be applied in the study of asymmetry arrangements of monomer units in polymers. It can reflect such physical properties as the elasticity, strength, and melting point of the polymer. These will be some of the properties that need to be understood when one tries to design polymers of specific characteristics. The weighted dissimilarity index might be of use in the analysis of protein–protein interaction networks. Using this, researchers could tell which of the proteins in the signaling pathway perform as critical hubs or bottlenecks. It is indicative of a specific role of these proteins in creating network asymmetry.

5.5. Biological Networks

Asymmetry of neural networks is important in neuroscience because it can provide further details on the functioning of different parts of a neural network in relation to each other. For example, what kind of specialization does the brain have? It is possible to map these differences with a weighted index of differences and then relate them to various cognitive processes or neurological disorders.

5.6. Graph Theory and Combinatorics

It can also be applied to problems of graph isomorphism where the aim would be to check if two graphs have the same structure. By providing a numerical quantity, it would be useful as a heuristic in an algorithm which will attempt to solve these problems. The weighted asymmetry index is graph-invariant; it does not change under the isomorphisms of graphs. This makes it useful for use as a tool in structural graph classification and in the identification of non-isomorphic graphs.

5.7. Optimization Problems

The weighted asymmetry index can be used in hedging for routing optimization within logistics and transportation networks, showing the asymmetries of that network by reducing them, hence bringing on efficient routing paths and reducing the cost of transportation. The weighted asymmetry index presents a way to analyze and improve the structure of the supply chain network for better distribution of resources and less bottleneck.

6. Conclusions

Theorems 1–6 provide crisp results and extremal values regarding the weighted asymmetry index on different families of graphs. Such results are important in demonstrating that the WA index exhibits structural sensitivity—a property that differentiates it from other popular topological indices, such as the Wiener index and the Szeged and Mostar indices. In the following Theorem 1, we will find out the extremal values of the WA index for trees and show that the star graph is a tree with the maximal value of WA, while the path graph has the minimum value of WA. This again underlines the fact that the WA index is sensitive

to asymmetry: Among the graphs, the star is the most asymmetric of its peripheral vertices at the maximum possible mutual distance, and the path is very symmetric; hence, WA is much smaller. Similarly, Theorem 2 shows the extremal values for unicyclic graphs. The result is an immediate application in chemical graph theory because unicyclic structures are common in molecular graphs. The WA index characterizes the imbalance in vertex distances more precisely than indices that cannot characterize such graphs as distinctly, for example, Wiener- or Szeged-type indices.

Similarly to the Wiener and Szeged indices, the weighted asymmetry index represents a distance-based topological index; its main advantage, however, is that it can describe structural asymmetries missed by other indices. For instance, the Wiener index is a summation of all the vertex pair distances, containing equal weighting for each vertex without regard for a local asymmetry near every edge. Although the Szeged index considers the local contributions by counting vertices on either side of an edge, the normalization with respect to the distances within the WA formula is not considered. However, the introduction of weights depending on inverse distances in the index makes the WA index a fine-tuned tool to describe the asymmetrical distribution of a graph's vertices around every given edge. That is why it is very useful in applications where local imbalance or asymmetry can play an important role, such as network vulnerability, molecular stability, or efficiency in communication.

It covers theorems that deal with graph families: bipartite, star, and wheel graphs, which are very common in network theory. For instance, in a bipartite graph, the WA index offers insight into how information may flow unequally between two sets of nodes, with an opportunity to provide a starting point for network design to make the flow equal or for various heuristics to be proposed. In the same manner, the wheel graphs are representative here to identify how centralization would encroach upon network asymmetry and offer a tool for resilience in a network against the failure of the hub.

These results touch on real-world applications in transportation networks and social graphs, where asymmetry usually implies some sort of inefficiency or vulnerability. Different from most of the classical connectivity indices, the WA index measures localized structural imbalances and hence enables optimizations on a much finer scale. At present, weighted asymmetry is a new contribution to graph theory, giving a different perspective to quantify and analyze asymmetries inside networks. Such an approach may also be highly useful in contexts where imbalance is decisive, such as in molecular graphs whose asymmetry is deemed to influence stability or in communication networks where asymmetrical topologies can provoke inefficiency and bottlenecks. In contrast to other well-known global indices, such as the sum of distances or centralities, the WA index offers a more local view that distinguishes graphs on the basis of their structural niceties. This gives it an edge over the existing indices in fields where such details are important.

Future investigations should be performed regarding extensive numerical simulations and case studies on real networks, such as social networks, biological networks, and communication networks, in order to empirically prove the practical benefits of the WA index over other indices. Applications will involve network vulnerability detection, anomaly detection, and efficiency optimization in order to find out its utility in highly dynamic and large-scale systems. Another very promising line of research involves an investigation into how the WA index can be further integrated into graph representation learning frameworks and machine learning models, especially in tasks where asymmetry plays a crucial role.

Moreover, the extremal values of the WA index for many classes of graphs remain open theoretically. The determination of the extremal graphs will allow a deeper insight into the structural implication brought by the WA index. We conclude, therefore, that a comparative study between the WA index and other centrality measures with regard to their prediction ability related to influential nodes in complex networks may be considered as an open problem that can inspire attention from researchers working in this area. These challenges, while adding to the understanding of the WA index, also extend its applicability in graph theory and network science.

Author Contributions: Conceptualization, A.N.A.K. and M.F.N.; methodology, M.F.N., A.A. and H.A.E.; validation, H.A.E., A.A. and M.F.N.; formal analysis, M.F.N., A.A. and A.N.A.K.; investigation, H.A.E., A.A. and M.F.N.; writing—original draft preparation, M.F.N. and A.N.A.K.; writing—review and editing, H.A.E. and M.F.N.; funding acquisition, A.N.A.K. All authors have read and agreed to the published version of the manuscript.

Funding: The authors gratefully acknowledge the funding of the Deanship of Graduate Studies and Scientific Research, Jazan University, Saudi Arabia, through project number RG24-L04.

Data Availability Statement: The data that support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest: The authors declare that they have no conflicts of interest.

References

1. Riaz, F.; Ali, K.M. Applications of graph theory in computer science. In Proceedings of the 2011 Third International Conference on Computational Intelligence, Communication Systems and Networks, Bali, Indonesia, 26–28 July 2011; pp. 142–145.
2. Majeed, A.; Rauf, I. Graph theory: A comprehensive survey about graph theory applications in computer science and social networks. *Inventions* **2020**, *5*, 10. [CrossRef]
3. Pavlopoulos, G.A.; Secrier, M.; Moschopoulos, C.N.; Soldatos, T.G.; Kossida, S.; Aerts, J.; Schneider, R.; Bagos, P.G. Using graph theory to analyze biological networks. *Biodata Min.* **2011**, *4*, 10. [CrossRef] [PubMed]
4. Trinajstic, N. *Chemical Graph Theory*; CRC Press: Boca Raton, FL, USA, 2018.
5. Bonchev, D. *Chemical Graph Theory: Introduction and Fundamentals*; Routledge: New York, NY, USA, 2018.
6. Gutman, I. Chemical graph theory—The mathematical connection. *Adv. Quantum Chem.* **2006**, *51*, 125–138.
7. Guze, S. Graph theory approach to the vulnerability of transportation networks. *Algorithms* **2019**, *12*, 270. [CrossRef]
8. Morro-Mello, I.; Padilha-Feltrin, A.; Melo, J.D.; Heymann, F. Spatial connection cost minimization of EV fast charging stations in electric distribution networks using local search and graph theory. *Energy* **2021**, *235*, 121380. [CrossRef]
9. Kostić, S.M.; Simić, M.I.; Kostić, M.V. Social network analysis and churn prediction in telecommunications using graph theory. *Entropy* **2020**, *22*, 753. [CrossRef]
10. Hansen, P.J.; Jurs, P.C. Chemical applications of graph theory. Part I. Fundamentals and topological indices. *J. Chem. Educ.* **1988**, *65*, 574. [CrossRef]
11. Estrada, E.; Uriarte, E. Recent advances on the role of topological indices in drug discovery research. *Curr. Med. Chem.* **2001**, *8*, 1573–1588. [CrossRef]
12. Gnanaraj, L.R.M.; Ganesan, D.; Siddiqui, M.K. Topological indices and QSPR analysis of NSAID drugs. *Polycycl. Aromat. Compd.* **2023**, *43*, 9479–9495. [CrossRef]
13. Hamid, K.; Waseem Iqbal, M.; Abbas, Q.; Arif, M.; Brezulianu, A.; Geman, O. Discovering irregularities from computer networks by topological mapping. *Appl. Sci.* **2022**, *12*, 12051. [CrossRef]
14. Javaid, M.; Cao, J. Computing topological indices of probabilistic neural network. *Neural Comput. Appl.* **2018**, *30*, 3869–3876. [CrossRef]
15. Liu, J.B.; Zhao, J.; Wang, S.; Javaid, M.; Cao, J. On the topological properties of the certain neural networks. *J. Artif. Intell. Soft Comput. Res.* **2018**, *8*, 257–268. [CrossRef]
16. Liu, J.B.; Zhang, T.; Wang, Y.; Lin, W. The Kirchhoff index and spanning trees of Möbius/cylinder octagonal chain. *Discret. Appl. Math.* **2022**, *307*, 22–31. [CrossRef]
17. Nadeem, M.F.; Ishfaq, F.; Shabbir, A. On Resistance Distance and Kirchhoff Index of Cacti Networks. *J. Stat. Phys.* **2024**, *191*, 83. [CrossRef]
18. Rücker, G.; Rücker, C. On topological indices, boiling points, and cycloalkanes. *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 788–802. [CrossRef]
19. Miličević, A.; Raos, N. Estimation of stability of coordination compounds by using topological indices. *Polyhedron* **2006**, *25*, 2800–2808. [CrossRef]
20. Basak, S.C. Information theoretic indices of neighborhood complexity and their applications. In *Topological Indices and Related Descriptors in QSAR and QSPR*; CRC Press: Boca Raton, FL, USA, 2000; pp. 573–604.
21. Basak, S.C.; Niemi, G.J.; Veith, G.D. Predicting properties of molecules using graph invariants. *J. Math. Chem.* **1991**, *7*, 243–272. [CrossRef]
22. Dehmer, M.; Emmert-Streib, F.; Shi, Y. Interrelations of graph distance measures based on topological indices. *PLoS ONE* **2014**, *9*, e94985. [CrossRef]
23. Zhang, X.; Reddy, H.G.; Usha, A.; Shanmukha, M.C.; Farahani, M.R.; Alaeiyan, M. A study on anti-malaria drugs using degree-based topological indices through QSPR analysis. *Math. Biosci. Eng.* **2023**, *20*, 3594–3609. [CrossRef]
24. Ullah, A.; Zaman, S.; Hussain, A.; Jabeen, A.; Belay, M.B. Derivation of mathematical closed form expressions for certain irregular topological indices of 2D nanotubes. *Sci. Rep.* **2023**, *13*, 11187. [CrossRef]

25. Gutman, I.; Furtula, B.; Oz, M.S. Geometric approach to vertex-degree-based topological indices–Elliptic Sombor index, theory and application. *Int. J. Quantum Chem.* **2024**, *124*, e27346. [CrossRef]
26. Hayat, S.; Khan, A.; Ali, K.; Liu, J.B. Structure-property modeling for thermodynamic properties of benzenoid hydrocarbons by temperature-based topological indices. *Ain Shams Eng. J.* **2024**, *15*, 102586. [CrossRef]
27. Huang, R.; Mahboob, A.; Rasheed, M.W.; Alam, S.M.; Siddiqui, M.K. On molecular modeling and QSPR analysis of lyme disease medicines via topological indices. *Eur. Phys. J. Plus* **2023**, *138*, 243. [CrossRef]
28. Arockiaraj, M.; Greeni, A.B.; Kalaam, A.A. Linear versus cubic regression models for analyzing generalized reverse degree based topological indices of certain latest corona treatment drug molecules. *Int. J. Quantum Chem.* **2023**, *123*, e27136. [CrossRef]
29. Ghani, M.U.; Campena, F.J.H.; Ali, S.; Dehraj, S.; Cancan, M.; Alharbi, F.M.; Galal, A.M. Characterizations of chemical networks entropies by K-banhatii topological indices. *Symmetry* **2023**, *15*, 143. [CrossRef]
30. Došlić, T.; Martinjak, I.; Škrekovski, R.; Tipurić, Spužević, S.; Zubac, I. Mostar index. *J. Math. Chem.* **2018**, *56*, 2995–3013. [CrossRef]
31. Zaman, S.; Kamboh, A.; Ullah, A.; Liu, J.B. Development of some novel resistance distance based topological indices for certain special types of graph networks. *Phys. Scr.* **2023**, *98*, 125250. [CrossRef]
32. Nagarajan, S.; Priyadharsini, G.; Pattabiraman, K. QSPR modeling of status-based topological indices with COVID-19 drugs. *Polycycl. Aromat. Compd.* **2023**, *43*, 6868–6887. [CrossRef]
33. Gao, F.; Xu, K.; Došlić, T. On the difference of Mostar index and irregularity of graphs. *Bull. Malays. Math. Sci. Soc.* **2021**, *44*, 905–926. [CrossRef]
34. Havare, O.C. Mostar Index (Mo) and edge Mo index for some cycle related graphs. *Rom. J. Math. Comput. Sci.* **2020**, *10*, 53–66.
35. Dinar, J.; Hussain, Z.; Zaman, S.; Rehman, S.U. Wiener index for an intuitionistic fuzzy graph and its application in water pipeline network. *Ain Shams Eng. J.* **2023**, *14*, 101826. [CrossRef]
36. Asmarani, E.Y.; Lestari, S.T.; Purnamasari, D.; Syarifudin, A.G.; Salwa, S.; Wardhana, I.G.A.W. The first zagreb index, the wiener index, and the gutman index of the power of dihedral group. *CAUCHY J. Mat. Murni Dan Apl.* **2023**, *7*, 513–520. [CrossRef]
37. Khadikar, P.V.; Karmarkar, S.; Varma, R.G. On the estimation of PI index of polyacenes. *Acta Chim. Slov.* **2002**, *49*, 755–772.
38. Ilić, A.; Milosavljević, N. The weighted vertex PI index. *Math. Comput. Model.* **2013**, *57*, 623–631. [CrossRef]
39. Barthelemy, M. Betweenness centrality in large complex networks. *Eur. Phys. J. B* **2004**, *38*, 163–168. [CrossRef]
40. Wiener, H. Structural determination of paraffin boiling points. *J. Am. Chem. Soc.* **1947**, *69*, 17–20. [CrossRef]
41. Gutman, I. A formula for the Wiener number of trees and its extension to graphs containing cycles. *Graph Theory Notes NY* **1994**, *27*, 9–15.
42. Khadikar, P.V. On a novel structural de-scriptor pi. *Natl. Acad. Sci. Lett.* **2000**, *23*, 113–118.
43. Brandes, U. A faster algorithm for betweenness centrality. *J. Math. Sociol.* **2001**, *25*, 163–177. [CrossRef]
44. Koschützki, D.; Lehmann, K.A.; Peeters, L.; Richter, S.; Tenfelde-Podehl, D.; Zlotowski, O. Centrality indices. In *Network Analysis: Methodological Foundations*; Springer: Berlin/Heidelberg, Germany, 2005; pp. 16–61.
45. Bloch, F.; Jackson, M.O.; Tebaldi, P. Centrality measures in networks. *Soc. Choice Welf.* **2023**, *61*, 413–453. [CrossRef]
46. Shimbel, A. Structural parameters of communication networks. *Bull. Math. Biophys.* **1953**, *15*, 501–507. [CrossRef]
47. Plavšić, D.; Nikolić, S.; Trinajstić, N.; Mihalić, Z. On the Harary index for the characterization of chemical graphs. *J. Math. Chem.* **1993**, *12*, 235–250. [CrossRef]
48. Ivanciuc, O.; Balaban, T.S.; Balaban, A.T. Design of topological indices. Part 4. Reciprocal distance matrix, related local vertex invariants and topological indices. *J. Math. Chem.* **1993**, *12*, 309–318.
49. Randić, M. Novel molecular descriptor for structure—Property studies. *Chem. Phys. Lett.* **1993**, *211*, 478–483. [CrossRef]

Disclaimer/Publisher's Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.