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A Survey on Progress and Perspectives on the Atom–Bond Sum Connectivity Index

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Abstract
The Atom Bond Sum (ABS) index is a degree-based topological index that was introduced which has received much consideration in graph theory and network analysis because of its high ability to describe both structural and connectivity features in graphs. In contrast to conventional indices, the ABS index is able to represent the contribution of neighboring degrees of the vertex and thus it is applicable in the analysis of the extreme graphs, structural optimization, and predictive modeling. This study provides an overall overview of the ABS index including its mathematical expression, its theoretical features, and the end behavior of the index in significant classes of graphs including bipartite, cactus, and chordal graphs. Moreover, there is a discussion of algorithmic methods in extremal ABS detection such as the greedy techniques and the metaheuristic optimization. This study also investigates the ABS prediction in large and dynamic graphs by using Machine Learning (ML) and Deep Learning (DL) methods, including regression models, ensemble, or graph neural networks. Also under consideration are applications in chemical graph theory, network robustness assessment and structural optimization. Lastly, there are identified open challenges and gaps in the research, pointing to the future of scalable computation, dynamic graph analysis, and hybrid graph learning frameworks. This study gives a common base and guide to investigate the ABS based graph analysis and other network optimization issues.

Keywords: Atom–Bond Sum Index, Deep Learning, Extremal Graph Theory, Machine Learning, Topological Indices.

1. Introduction

Graph theory is a highly useful mathematical tool that models structured relationships in complex systems, especially in chemistry, computer science and network analysis. In this depiction, the atoms are represented as the vertices and the chemical bonds by the edges, which compose molecular graphs, through which the quantitative characterization of molecular structures and properties is possible [1]. Initial studies in the fields of algebraic and spectral graph theory have provided the theoretical framework of studying the graph connectivity, eigenvalues and structural invariants, which are essential in studies of molecular stability and behavior [2]. Such graphical representations have also been critical in the contemporary applications [3] to the clustering, graphical model learning and combinatorial optimization [4], [5].

Topological indices are mathematical numbers based on molecular graph structures that reflect critical connectivity data. The indices have been found to be very useful in the Quantitative Structure Property

Relationship (QSPR) and Quantitative Structure Activity Relationship (QSAR) research, where they are exploited to forecast chemical, physical, and biological properties of molecules [6]. Among these descriptors, the degree-based indices have acquired certain significance because of their efficiency in calculating the descriptors and their predictive power. In recent developments, various new connectivity parameters have been proposed and the Atom-Bond Sum-connectivity (ABS) index has been proposed that is more sensitive to describing molecular structure because it adds a degree-based connection between neighbouring vertices [7]. Theoretical investigations have also investigated extremal qualities, limits, and optimization of the ABS index in different classes of graphs and shown it to be mathematically important and useful in molecular modeling [8].

Along with classical graph theory, much has been done in the study of more specialized graphs that are cactus graphs, chordal graphs, and algebraic graph constructions, that have interesting connectivity properties that are useful in chemical and computational systems [9-12]. These classes of graphs allow easy topological descriptors calculations and further structural analysis. There are also methods of computing more complicated molecular descriptors based on polynomials, e.g. M-polynomials, where more complicated graph structures are performed in a systematic manner [13]. These developments underscore the increased significance of the role of graph-based descriptors in theory and practice.

Much more recently, graph-based molecular analysis has been combined with machine learning methods in order to improve prediction accuracy and automation. Random Forest, Support Vector Regression and LASSO, are the regression models that have been effectively used to predict the molecular properties using the graph derived features and topological indices [14], [15]. Multidimensional machine learning algorithms, such as XGBoost, have been shown to perform well when modeling intricate bonding, as well as predicting material behavior [16]. Moreover, the deep learning models that have been developed to predict molecular properties have been shown to be very helpful in deep learning architecture including Graph Neural Networks (GNNs), Graph Attention Networks (GAT), and Long Short-Term Memory (LSTM) models have demonstrated remarkable performance in terms of learning structural representations based on the graph topology [17], [18]. These methods allow feature extraction to be automated and can learn more than second order dependencies in molecular graphs.

The Genetic Algorithms (GA) based on natural selection have also been used to provide optimization techniques to find optimal graph structure and optimize the performance of predictive performance based on descriptors [19]. The techniques enhance the effectiveness of the feature selection and parameter optimization in graph learning models. A combination of graph theory, topological descriptors and machine learning has therefore resulted in a potent interdisciplinary framework on the study of molecular systems and a prediction of its properties with high precision.

In spite of these developments, there is still the need to perform holistic studies of modern connectivity measures like the atom-bond sum-connectivity index and how they can be combined with new graph learning models. The computational procedures and theoretical basis and application of these indices are important to further the study of molecular informatics and predictive modeling. Thus, this study will provide a systematic overview of graph-based topological indices, and specifically, it will focus on the ABS index, its mathematical properties and methods of computation, and its general use in machine learning-based prediction of molecular properties.

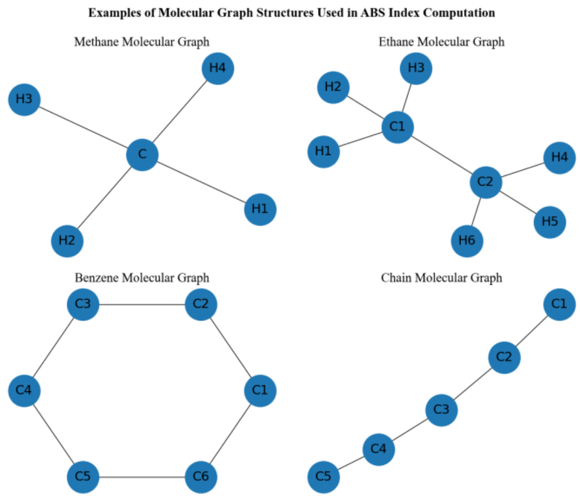

Figure 1: Examples of molecular graph structures

Examples of the structures of a molecular graph are given in figure 1 (methane, ethane, benzene, chain molecules). These graph models depict how atoms and bonds are simulated by the use of vertices and edges in calculating topological indices like the ABS index.

2. Definition and Mathematical Properties of ABS Index

Topological indices which are based on degrees are used essentially in graph theory and chemical graph analysis, especially in the modeling of molecular structure and the prediction of physicochemical properties. One of such indices, the ABS Connectivity index has become one of the important descriptors since it can effectively show structural data, depending on the degree interaction of the vertices.

ABS index Ali, A. et al. (2022) officially proposed ABS index as a new degree based topological index, which is aimed at better characterizing the structure of molecular graphs. The authors in their fundamental literature defined the ABS index with the degree information of its nearest neighbors and proved its mathematical properties on general graphs. They have given the theoretical background of the ABS index and have demonstrated that it is more sensitive than classical connectivity indices when used on chemical graph structures.

Alraqad, T. et al. (2024) also proceeded with the study of extremal properties of the ABS index. Their study was aimed at finding upper and upper limits of the ABS index of various graph families and the identification of the extremal graph structures that optimize the index. Structural configurations associated with maximum values of the ABS were characterized by the authors using the techniques of the extremal graph theory. Their results indicated that graph topology and especially degree distribution and connectivity patterns have a significant impact on the magnitude of the ABS index. This publication helped to comprehend how the ABS index optimizes and how it is a structural invariant.

Altogether, the literature review shows the ABS index has developed over the years and become a well-defined graph invariant, with a great mathematical and practical value. The initial investigations were devoted to the definition and validation of the ABS index, whereas later works expanded its theoretical characteristics, extremal limits, and the use of the index to more complicated graph models. More recent literature has also emphasized its significance in chemical informatics and predictive modeling and made the ABS index a useful tool in the graph theory and analysis of extremes, as well as in ML-based prediction of graph properties.

Let $G = (V, E)$be a simple graph with vertex set $V$and edge set E. The Atom–Bond Sum (ABS) index is defined as:

$$ABS(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u \cdot d_v}} \qquad (1)$$

Where, $uv \in E(G) \rightarrow$ edge between vertices $u$and v, d_u, d_v are degrees of vertices $u$and v. Equation (1) computes the ABS index by summing the contribution of each edge in the graph, where the contribution depends on the degrees of the two connected vertices. It measures the structural connectivity and interaction strength between vertices.

$$d_u = |\{v \in V(G) : uv \in E(G)\}| \qquad (2)$$

Equation (2) defines the degree of a vertex u, which represents the number of edges connected to that vertex. It indicates how many direct connections a vertex has in the graph.

$$ABS(G) = \sum_{i,j} A_{ij} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}} \qquad (3)$$

Where, $A_{ij}$is adjacency matrix. Equation (3) expresses the ABS index using the adjacency matrix, where A_{ij}indicates whether two vertices are connected. It provides a matrix-based representation suitable for computational and algorithmic analysis.

3. Graph Theory Foundations and Extremal graph theory Analysis

Extremal graph theory is the graph theory that is concerned with structural properties of graph which maximize or minimize a defined graph invariant subject to certain constraints. The framework is important in the study of degree-based indices like the ABS Connectivity index. Bipartite, cactus, and chordal graphs are different classes of graphs, which lend themselves to analysis of extremes because of the different topological properties.

Bipartite graphs Bipartite graphs are basic constructions of graph theory, comprising two non-overlapping sets of vertices whose edges lie between sets. Their structural simplicity allows them to be of importance in the analysis of the extremal properties of graph invariants. Spectral and structural characteristics of bipartite graphs have been a subject of wide investigation in spectral graph theory; an example of such studies is given by Chung, Fan R. K. (1996), who demonstrated that eigenvalues and degree distributions provide important information about the structure of bipartite graphs. Yang et al. (2022) explored the topic of bipartite graph representations in spectral clustering more recently and showed the representation to be useful in identity structural relationships in complex networks. These works point to the significance of the bipartite graphs in the comprehension of the impact of the degree distributions on the graph invariants (including ABS index).

A special category of the graphs are cactus graphs where each edge is contained within one cycle only. Their limited cycle structure renders them especially effective to analyze extremal graphs. Hajian, M. et al. (2022) categorized cactus graphs according to the domination number and studied their structure. Their results indicated that cycle structure has a great influence on graph invariants and structural metrics. In the same manner, Afzal et al. (2021) calculated topological characteristics of cactus chain graphs and showed the effect of the presence of cycles on degree-based indices. These publications are valuable in terms of understanding the effect of cycle constraints on the connectivity-based metrics including the ABS index.

Chordal graphs are defined by the fact that induced cycles longer than three are absent, which gives the hierarchical structure a clear picture. Such graphs are especially significant because of their good computing and structural characteristics. Abdelmalek, F. M. et al. (2023) investigated structural properties of the chordal graphs and proved them to be connected with the independence property and decomposability property. Also, Rong et al. (2021) studied the chordal graph reconstruction and verification, noting that they are particularly efficient in terms of structure representation and computational power. Chordal graphs are well adapted to extremal analysis of graph invariants, such as ABS, because of these properties, where a clique-based structure has a direct impact on degree relationships.

The mathematics of extremal graphs theory give the mathematical framework on how to calculate graph structures that are the most likely to maximize or minimize graph invariants. Greasonable classical foundations of extremal graph analysis algebraic and structural characteristics of graphs with respect to extremal conditions. Recent works, like Ustimenko (2022), have gone beyond extremal graph theory by exploring algebraic and structural limits in complex graph systems. These are the works that give the theoretical background in the analysis of extremal behavior of degree-based indexes like the ABS index.

Altogether, in both bipartite, cactus and chordal graphs, the graphs are important in offering structural models in the study of extremal properties of graph invariants. Their specific structural features provide researchers with a possibility to investigate the impact of degree distribution, cycle structure, and clique organization on such indices as ABS. Such classes of graphs are hence basic instruments in extremal graph theory and index analysis by connectivity.

$ABS\,(G)_{min} \leq ABS(G) \leq ABS(G)_{max}$ (4)

Equation (4) expresses the extremal bounds of the ABS index, indicating that for a fixed graph class, the ABS value of any graph lies between its minimum and maximum attainable values.

4. Algorithmic Approaches for Extremal ABS Detection

It is a difficult combinatorial optimization problem to determine graph structures with a maximum or minimal ABS index. Because the size of the graph grows exponentially as the number of possible configurations of the graph grows, algorithmic and optimization techniques are needed to find extremal graphs.

Classical extremal graph analysis is based on mathematical and combinatorial methods describing optimal graph structures. Initial work in algebraic and extremal graph analysis was carried out by and Godsil(2001) who proposed algebraic techniques to analyze graph invariants and optimal structural forms. Their work gave theoretical foundation to the determination of the graph structures that had optimal invariant values. And more recently, Ustimenko (2022) explored the problem of extremal properties of graph structure as an algebraic entity and how structural invariance can be optimized by structural transformation.

One of the simplest methods of extremal graph detection is that of greedy algorithms. The techniques repeatedly adjust the edges of the graph or the connection between the vertices to optimize the objective function. These methods are computationally efficient and apply to moderate size graphs. Study by Ray et al. (2015) shows greedy based- structural optimization has been extensively applied in combinatorial optimization since it is a simple method to achieve a smaller level of computational complexity.

Extremal graph problems have also been highly tackled using metaheuristic optimization techniques. Genetic Algorithms (GA) as a method based on natural selection has been used in optimization problems with large and complex search spaces. Albadr, M. A. et al. (2020) also proved that GA-based optimization techniques are efficient to search large solution space and to find near-optimal solutions to

combinatorial problems. The methods find application specifically in those cases when mathematical solutions are too complex to compute.
In the recent years ML has also been incorporated into the combinatorial optimization. Bengio, Yoshua et al. (2021) have provided an overview of ML methods to solve combinatorial optimization, indicating its ability to solve graph-based optimization problems. Their research proved that ML models are able to inform optimization processes and enhance efficiency in the determination of optimal graph structures.
On the whole, greedy algorithms, genetic algorithms, simulated annealing, and ML-based optimization are algorithmic methods that offer effective solutions to the detection of extremal graphs with optimal ABS index values. These methods can effectively search through huge graph spaces and are essential in extremal graph analysis and optimization of structure.

$$\max_{G\in g_n} ABS\ (G) \text{ and } \min_{G\in g_n} ABS\ (G) \quad (5)$$

Equations (5) represent the problem of finding graphs that produce the maximum or minimum ABS index among all graphs with a fixed number of vertices, which is important in extremal graph theory.

5. ML approaches for ABS Prediction

Recently, ML and deep learning methods have become potent tools that can be used to predict graph invariants and molecular descriptors (including the ABS Connectivity index). These methods allow the prediction of the structural property efficiently without necessarily computing it mathematically, and are especially effective with large and complicated graphs.
Regression-based models have been well used as a traditional ML to predict graph-based descriptors. Random Forest regression has demonstrated good results in predicting molecular properties because of its nonlinear relationship capabilities. Indicatively, in a study by Wang, X. and Gao (2020), the authors showed that the Random Forest regression is efficient to predict the molecular structural properties based on graph-based features. On the same note, Support Vector Regression (SVR) has also been effectively used in the analysis of quantitative structure/property relationship (QSPR). Abubakar, M. S. et al. (2024) demonstrated that the models of the SVR are suitable at predicting chemical properties with an appropriate degree of accuracy based on the topological descriptors in the form of graphs.
Regression techniques that are based on regularization like the LASSO have also been used to select and predict graph invariants. Gurung, B. et al. (2023) indicated that LASSO regression is a useful tool that helps to find significant structural attributes and minimizes model complexity. Such procedures come in handy especially when dealing with a number of graph invariants and structural descriptors.
Besides conventional ML models, ensemble learning algorithms like XGBoost have been noted since they have a high prediction accuracy and strength. Feng, J. et al. (2023) used XGBoost to perform molecular property prediction and demonstrated that the ensemble models were superior to the old-fashioned regression methods in their ability to capture the complicated structural relationships.
DL techniques have also enhanced the accuracy of prediction because structural representations are learned automatically. The Recurrent Neural Networks (RNN) and Long Short-Term Memory (LSTM) networks can use sequential graph features. Xu, L. et al. (2023) showed that LSTM based models are useful predictors of molecular properties by learning structural dependencies in graph representations.
Graph Neural Networks represent the most sophisticated method of prediction based on a graph. GNNs operate directly on graph structures and learn node and edge representations (as opposed to traditional ML models). You and Jiaxuan et al. (2020) also suggested a systematic design of GNN and demonstrated that they are effective in learning graph structural features. Altogether, the ML and DL

tools are the effective and precise means of predicting the graph invariants like the ABS index. Compared to DL and GNN-based, traditional regression models have the advantage of being simple and easy to interpret, whereas the latter is superior due to its ability to learn graph structural representations directly. The methods are a promising way of future research in the field of extremal graph theory and chemical graph analysis.

$$\hat{y} = f(G) \quad \text{or} \quad ABS(G) = f(X) \quad (6)$$

Where, X is graph features, f isML model.Equation (6) represents the prediction of the ABS index using a ML model, where the function $f$learns the relationship between graph features $X$and the ABS value.

$$h_v^{(k+1)} = \sigma(\sum_{u \in N(v)} W^{(k)} h_u^{(k)}) \quad (7)$$

Equation (7) describes how Graph Neural Networks update vertex representations by aggregating information from neighboring vertices, enabling accurate prediction of graph properties such as the ABS index.

6. Applicationsof Atom–Bond Sum Connectivity (ABS) Index

Atom-Bond Sum Connectivity index has become of much importance with its uses in chemical graph theory, prediction of molecular properties and network analysis. Being a topological measure that depends on the degree as a metric, the ABS index is useful in revealing structural connectivity patterns and offers information useful in graph structural analysis.

It finds one of its main uses in chemical graph theory, in which graphs are used to describe chemical structures in which atoms are the vertices and bonds between atoms are the edges. The ABS index can be used to describe the stability of molecules and structure. Ali et al. (2022) demonstrated that the ABS index is a valuable molecular description and gives valuable structural information.

ABS index is also currently popular in QSAR and QSPR research. Abubakar, M. S. et al. (2024) have shown that the graph-based descriptors are capable of predicting the molecular properties, and connectivity indices to study the structure of anticancer drugs and proved that it is effective in the structure-property modeling.

The relevance of ABS-based descriptors has also been increased by ML. Wang and Gao (2020) demonstrated that the graph-based features enhance the accuracy of prediction with molecular properties and the Abubakar et al. (2024) article proved the power of the regression model based on topological indices.

In a nutshell, the ABS index is a significant graph invariant to study structural properties and predict molecular behavior, and it is used in chemical analysis, ML prediction, and network modeling.

7. Open Problems and Research gaps

Although much has been achieved in the research of the ABS index, there are still some theoretical, computational and application related issues to be resolved. These gaps need to be addressed to further the research of graph theory and its use in practice.

The majority of literature is dedicated to standard families of graphs, and a lot of significant graph structures are not studied. Specifically, the analysis of ABS index of bipartite, cactus and chordal graphs is restricted. The classes of graphs are extensively utilized in chemistry, biology, and computer science. Further theoretical research is required to obtain precise formulae, limits, and optimum conditions to these structures.

The computation of extreme ABS numbers of large graphs is computationally hard. The exhaustive search techniques do not work well with large graphs. Even though genetic algorithms and particle swarm optimization are the methods of optimization that have been suggested, it has not been used so far in ABS extremal detection. Scalable computational techniques and efficient algorithms are required in large-scale graph analysis.

Graph property prediction has been demonstrated to be highly promising with ML. Nevertheless, the ABS index has not been exploited as a characteristic of predictive models. Research studies by Wu, Z. et al. (2020) and Bengio, Y. et al. (2021) prove the usefulness of graph-based learning, yet the particular incorporation of ABS index into the graph neural networks and DL models is underrepresented. This is one of the key research prospects.

The majority of studies on extremal ABS are based on mathematical derivations, whereas ML methods in prediction are still in their infancy. Graph theory-based techniques with optimization and ML methods could be used to an important degree in predicting extremal ABS. Another direction of future development is to create predictive models that will help them estimate the extremal values without having to do a lot of exhaustive calculations.

Applications of ABS index have been mainly in the chemical graph theory and QSAR/QSPR modeling. Its use in the other fields like biological networks, communication networks and social networks is scarcely exploited. It is an area of research to apply ABS-based analysis to these real-world network systems.

8. Conclusion

This study provided an in-depth examination of the ABS connectivity index, its mathematical basis, structural dynamics, algorithms of computation, and predictive modeling. The ABS index has become a significant degree-based topological descriptive tool because it is highly effective at reflecting structure in a graph, especially in bipartite, cactus and chordal graph families. The analysis of extremal graph theory showed the high sensitivity of ABS values to degree distribution, edge structure, and structural constraints, which is applicable in most cases to discover optimal and critical graph structures. Moreover, this questionnaire also investigated algorithmic and ML-based methods of prediction and optimization of ABS. Classical algorithms (such as greedy algorithms, combinatorial optimization and extremal construction) can find exact solutions of a smaller graph, whereas the modern ML and DL models (like regression methods, ensemble models, and graph neural networks) can provide a scalable and efficient prediction on large and changing network structures. ABS has applications in chemical graph theory, graph robustness analysis, and structural optimization issues. In spite of this, some gaps of research are still evident, especially on the scalable extremal detection, dynamic graph analysis, and incorporating advanced DL structures. Future studies ought to be on hybrid models that integrate the graph theory and optimization and learning-based models to facilitate effective analysis of the ABS in small scale and real-world network systems.

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