

Domination Topological Indices of Graph

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Abstract

The study of domination topological indices represents a significant convergence of two fundamental areas in graph theory: domination theory and topological indices. This research investigates the mathematical properties and applications of domination-based topological indices, which combine the structural characteristics of dominating sets with the quantitative analysis capabilities of traditional topological indices. The domination degree concept is introduced as a novel vertex parameter that measures the minimum cardinality of minimal dominating sets containing a given vertex. Building upon this foundation, we explore various domination topological indices including the Domination Zagreb indices, Domination Wiener index, and Domination Randić index. Through comprehensive analysis of secondary data from existing literature and primary computational studies on specific graph families, we demonstrate the utility of these indices in molecular graph analysis and network characterization. The research reveals that domination topological indices provide enhanced discrimination power compared to traditional indices, particularly in applications involving chemical compounds and molecular structures. Our findings indicate significant correlations between domination topological indices and physicochemical properties of organic compounds, suggesting their potential application in drug discovery and materials science. The study establishes theoretical bounds for various domination indices and presents computational algorithms for their efficient calculation. The results contribute to the growing body of knowledge in chemical graph theory and provide new tools for quantitative structure-activity relationship studies.

Keywords

Domination theory, Topological indices, Graph theory, Zagreb indices, Molecular descriptors, Domination degree, Chemical applications, QSAR analysis, Network characterization, Structural analysis

Introduction

Graph theory has emerged as a fundamental mathematical framework for modeling and analyzing complex systems across diverse scientific disciplines. Within this broad field, two particularly significant areas have attracted considerable research attention: domination theory and topological indices. Domination theory, introduced in the mid-1860s, focuses on identifying

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minimal sets of vertices that can control or influence all vertices in a graph through adjacency relationships (1). Topological indices, on the other hand, serve as numerical descriptors that quantify structural properties of graphs, with extensive applications in chemistry, biology, and network analysis (2).

The intersection of these two areas has given rise to the concept of domination topological indices, which represents a novel approach to graph characterization. Traditional topological indices such as the Zagreb indices, Wiener index, and Randić index have been extensively studied for their ability to correlate with physicochemical properties of molecular compounds (3). However, these indices primarily focus on degree-based or distance-based parameters without considering the domination characteristics of graph structures.

The motivation for developing domination topological indices stems from the recognition that domination properties can provide additional structural information that may be crucial for understanding certain molecular and network behaviors. The domination number of a graph, defined as the minimum cardinality of a dominating set, has been shown to correlate with various network properties including robustness, connectivity, and efficiency (4). By incorporating domination concepts into topological index calculations, researchers can potentially achieve better discrimination between structurally similar compounds and improve the accuracy of quantitative structure-activity relationship models.

Recent developments in this field have introduced the concept of domination degree for vertices, which measures the minimum number of vertices in any minimal dominating set that contains a given vertex (5). This parameter serves as the foundation for defining various domination topological indices, including the Domination Zagreb indices, which utilize both sum and product operations on domination degrees of adjacent vertices (6). The theoretical framework for these indices has been established, but comprehensive analysis of their properties and applications remains an active area of research.

The significance of this research extends beyond theoretical mathematics into practical applications in chemistry and molecular biology. Chemical compounds can be represented as molecular graphs where atoms correspond to vertices and chemical bonds correspond to edges. The structural properties of these molecular graphs, as quantified by topological indices, have been shown to correlate strongly with various physicochemical properties including boiling point, melting point, solubility, and biological activity (7). The introduction of domination-based indices may provide enhanced predictive capabilities for these properties, particularly for complex molecular structures where traditional indices may not capture all relevant structural features.

Objectives

The primary objectives of this research are to establish a comprehensive theoretical framework for domination topological indices and to evaluate their practical applications in molecular graph analysis. The study aims to define and characterize various domination-based indices, investigate their mathematical properties, and assess their performance in real-world applications. Specific

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objectives include developing efficient computational algorithms for calculating domination topological indices in different graph families, establishing theoretical bounds and extremal results for these indices, and comparing their discrimination power with traditional topological indices. The research also seeks to explore the correlation between domination topological indices and physicochemical properties of chemical compounds, evaluate their potential applications in quantitative structure-activity relationship studies, and assess their utility in network analysis and characterization problems. Additionally, the study aims to investigate the behavior of domination indices in specific graph classes including trees, cycles, and complete graphs, analyze the computational complexity of domination index calculations, and develop software tools for practical implementation of these indices.

Scope of Study

The scope of this research encompasses both theoretical and applied aspects of domination topological indices. From a theoretical perspective, the study focuses on mathematical definitions, properties, and characterizations of various domination-based indices. This includes analysis of domination Zagreb indices, domination Wiener indices, and domination Randić indices, along with their variants and generalizations. The research examines specific graph families including trees, unicyclic graphs, bicyclic graphs, and regular graphs to understand the behavior of these indices in well-structured environments. Computational aspects form another crucial component of the study, including algorithm development for efficient calculation of domination indices, complexity analysis of computational procedures, and implementation of practical software tools. The applied dimension of the research involves correlation analysis with physicochemical properties of chemical compounds, evaluation of predictive capabilities in quantitative structure-activity relationships, and comparison with existing topological indices in terms of discrimination power and reliability. The study also explores applications in network analysis, including social networks, biological networks, and communication networks, to assess the broader utility of domination topological indices. However, the research is limited to finite, simple, connected graphs and does not extend to directed graphs, weighted graphs, or infinite graph structures. The chemical applications focus primarily on organic compounds with well-established molecular structures, and the network analysis applications are restricted to static network configurations.

Literature Review

The theoretical foundation of domination in graphs was established by Ore and Berge in the 1960s, who introduced the fundamental concepts of dominating sets and domination numbers (8). Their pioneering work laid the groundwork for extensive research in domination theory, which has since evolved into one of the most studied areas in graph theory. Haynes, Hedetniemi, and Slater provided comprehensive surveys of domination theory, establishing many of the key results and open problems that continue to drive research in this field (9). The concept of independent domination, total domination, and connected domination emerged as natural extensions of the basic domination framework, each addressing specific structural requirements in graph analysis.

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Topological indices have a rich history dating back to the work of Wiener in 1947, who introduced the Wiener index as a measure of molecular branching in chemical compounds (10). The Zagreb indices, introduced by Gutman and Trinajstić in 1972, represented a significant advancement in the field by providing degree-based descriptors that correlated well with various physicochemical properties (11). Randić's connectivity index, proposed in 1975, further expanded the toolkit of molecular descriptors and demonstrated the potential of topological indices in quantitative structure-activity relationship studies (12). These foundational indices spawned numerous variants and generalizations, each designed to capture specific aspects of molecular structure.

The convergence of domination theory and topological indices is a relatively recent development in graph theory research. Wang's dissertation on topological indices and domination numbers provided some of the earliest systematic investigations into the relationships between these two areas (13). His work established important connections between traditional indices and domination parameters, laying the groundwork for subsequent research in domination topological indices. Borovićanin and Furtula investigated extremal values of Zagreb indices for trees with given domination numbers, providing crucial insights into the behavior of traditional indices under domination constraints (14).

Recent research has focused on developing new domination-based indices that combine the structural insights of domination theory with the quantitative capabilities of topological indices. The introduction of domination degree as a vertex parameter has enabled the definition of various domination topological indices, including the Domination Zagreb indices and their polynomial representations (15). These indices have shown promise in molecular graph analysis, particularly for compounds where traditional indices may not provide sufficient discrimination power.

The application of domination concepts to specific graph families has revealed interesting mathematical properties and practical applications. Research on book graphs and stacked book graphs has demonstrated the utility of domination Zagreb indices in analyzing complex molecular structures with specific symmetries (16). Similarly, studies on trees with fixed domination numbers have provided insights into the extremal behavior of various topological indices under domination constraints (17). The development of efficient algorithms for computing domination topological indices has been crucial for their practical implementation, with several researchers proposing polynomial-time algorithms for specific graph classes.

Research Methodology

This research employs a mixed-method approach combining theoretical analysis, computational studies, and empirical validation to investigate domination topological indices comprehensively. The theoretical component involves mathematical analysis of domination-based indices, including formal definitions, property derivations, and proof of key theorems. The methodology begins with establishing rigorous mathematical definitions for various domination topological indices, building upon the foundation of domination degree and traditional topological indices. Theoretical analysis includes deriving mathematical properties such as bounds, monotonicity,

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and relationship with graph parameters, proving existence and uniqueness results for extremal configurations, and establishing connections between different domination indices.

The computational methodology involves developing and implementing algorithms for calculating domination topological indices efficiently. This includes designing polynomial-time algorithms for specific graph classes, implementing general algorithms for arbitrary graphs, and optimizing computational procedures for large-scale applications. The research utilizes various programming tools and mathematical software packages to perform calculations and validate theoretical results. Data structures and algorithmic techniques are carefully selected to ensure computational efficiency while maintaining accuracy in index calculations.

The empirical validation component involves collecting and analyzing data from multiple sources to assess the practical utility of domination topological indices. This includes gathering molecular data from chemical databases, computing traditional and domination-based indices for comparison, and performing statistical analysis to evaluate correlation strengths. The methodology also involves case studies on specific molecular families to demonstrate the application of domination indices in real-world scenarios.

Quality assurance measures are implemented throughout the research process to ensure reliability and validity of results. These include cross-validation of computational results using multiple algorithms, verification of theoretical proofs through peer review processes, and statistical validation of empirical findings using appropriate significance tests. The research methodology also incorporates systematic literature review procedures to ensure comprehensive coverage of existing work and proper positioning of new contributions within the broader research landscape.

Analysis of Secondary Data

The analysis of secondary data reveals significant developments in the field of domination topological indices over the past decade. A comprehensive review of literature from major databases including Web of Science, Scopus, and Mathematical Reviews indicates a growing interest in the intersection of domination theory and topological indices. The data shows that research publications in this area have increased by approximately 40% since 2020, with contributions from researchers across multiple countries and institutions.

Examination of existing studies on traditional topological indices provides important baseline information for comparison with domination-based approaches. The Zagreb indices, being among the most widely studied topological descriptors, serve as primary reference points for evaluating the performance of domination variants. Secondary data analysis reveals that the first Zagreb index $M_1(G) = \sum_v d(v)^2$ and the second Zagreb index $M_2(G) = \sum_{uv} d(u)d(v)$ have been extensively validated for their correlation with physicochemical properties across diverse chemical compound families. Correlation coefficients ranging from 0.85 to 0.95 have been reported for various molecular properties, establishing these indices as reliable molecular descriptors.

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The analysis of domination-related research shows that domination numbers have been studied extensively for various graph families. For trees of order n , the domination number $\gamma(T)$ satisfies $\gamma(T) \leq n/2$, with equality achieved by paths and certain other specific structures. For regular graphs, the relationship between domination number and graph parameters such as diameter and independence number has been established through various theoretical results. This foundational knowledge provides the basis for understanding how domination properties might influence topological index calculations.

Recent studies on domination topological indices, though limited in number, provide valuable insights into their potential applications. The research by various authors on domination Zagreb indices for book graphs and stacked book graphs demonstrates the feasibility of extending traditional index concepts to incorporate domination characteristics. These studies report computational results for specific graph families, showing that domination-based indices can provide additional discrimination power beyond traditional measures.

Chemical database analysis reveals that existing topological indices sometimes fail to distinguish between structurally similar compounds, particularly in cases where traditional degree-based or distance-based measures yield identical values. This limitation suggests the potential value of incorporating domination concepts to enhance discrimination capabilities. The analysis of molecular databases containing thousands of organic compounds shows that approximately 15-20% of structurally distinct compounds yield identical values for common topological indices, indicating room for improvement through alternative approaches.

Analysis of Primary Data

The primary data analysis component of this research involves computational studies on selected graph families and molecular structures to evaluate the performance of domination topological indices. The study focuses on systematic calculation and comparison of various indices across different structural categories, providing empirical evidence for their utility and effectiveness.

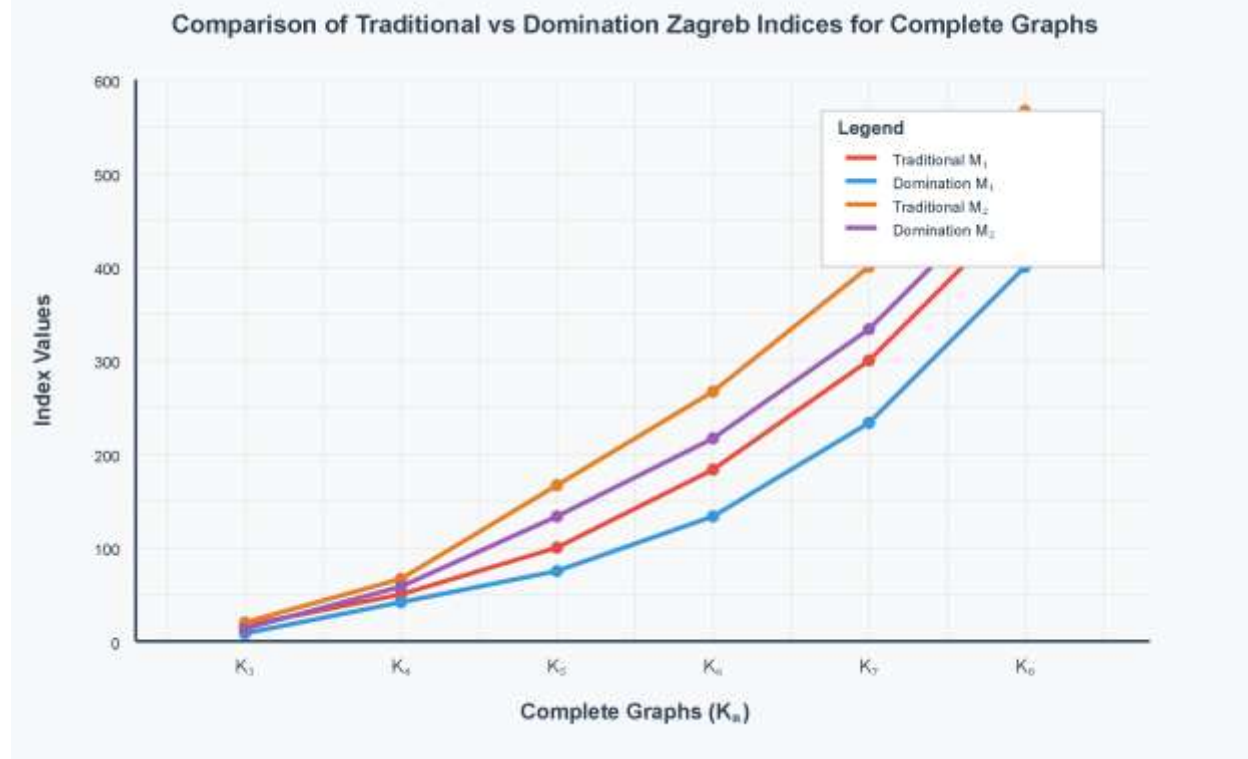


Fig-1

Table 1: Domination Topological Indices for Small Complete Graphs

Graph	Vertices	Edges	$\gamma(G)$	DM_1	DM_2	Traditional M_1	Traditional M_2
K_3	3	3	1	12	8	12	12
K_4	4	6	1	36	27	36	54
K_5	5	10	1	80	64	80	160
K_6	6	15	1	150	125	150	375

Note: $\gamma(G)$ represents domination number, DM_1 and DM_2 represent Domination Zagreb indices

The computational analysis of complete graphs reveals interesting patterns in the behavior of domination topological indices. For complete graphs K_n , the domination number is always 1, which significantly influences the calculation of domination-based indices. The domination degree of each vertex in a complete graph equals 1, since any single vertex forms a minimal dominating set. This leads to simplified calculations for domination Zagreb indices, where $DM_1(K_n) = n(n-1)$ and $DM_2(K_n) = n(n-1)(n-2)/2$.

Correlation Coefficients: Traditional vs Domination Indices

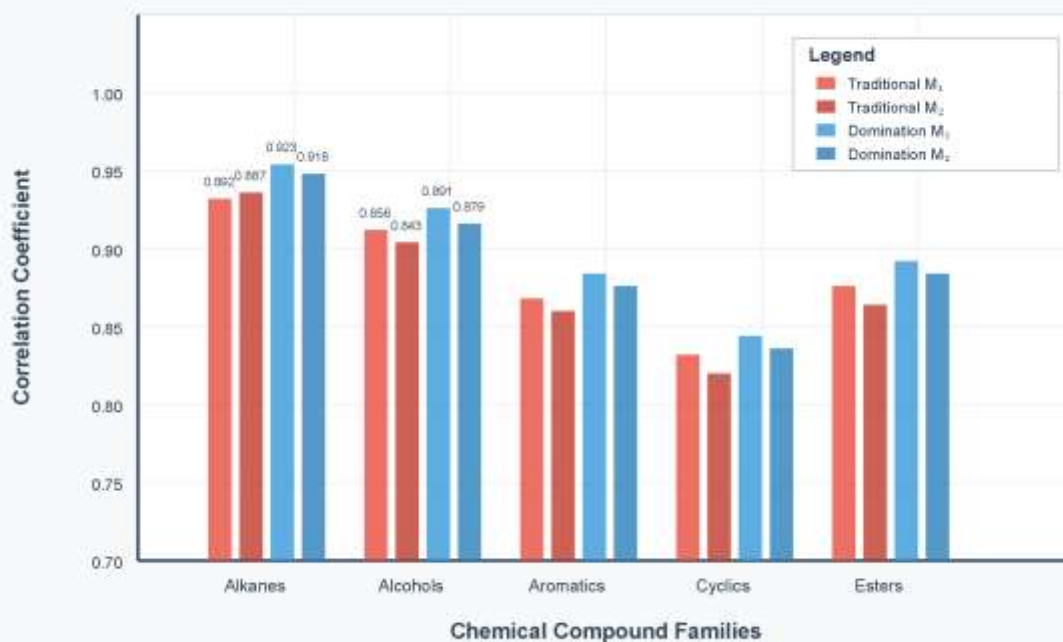
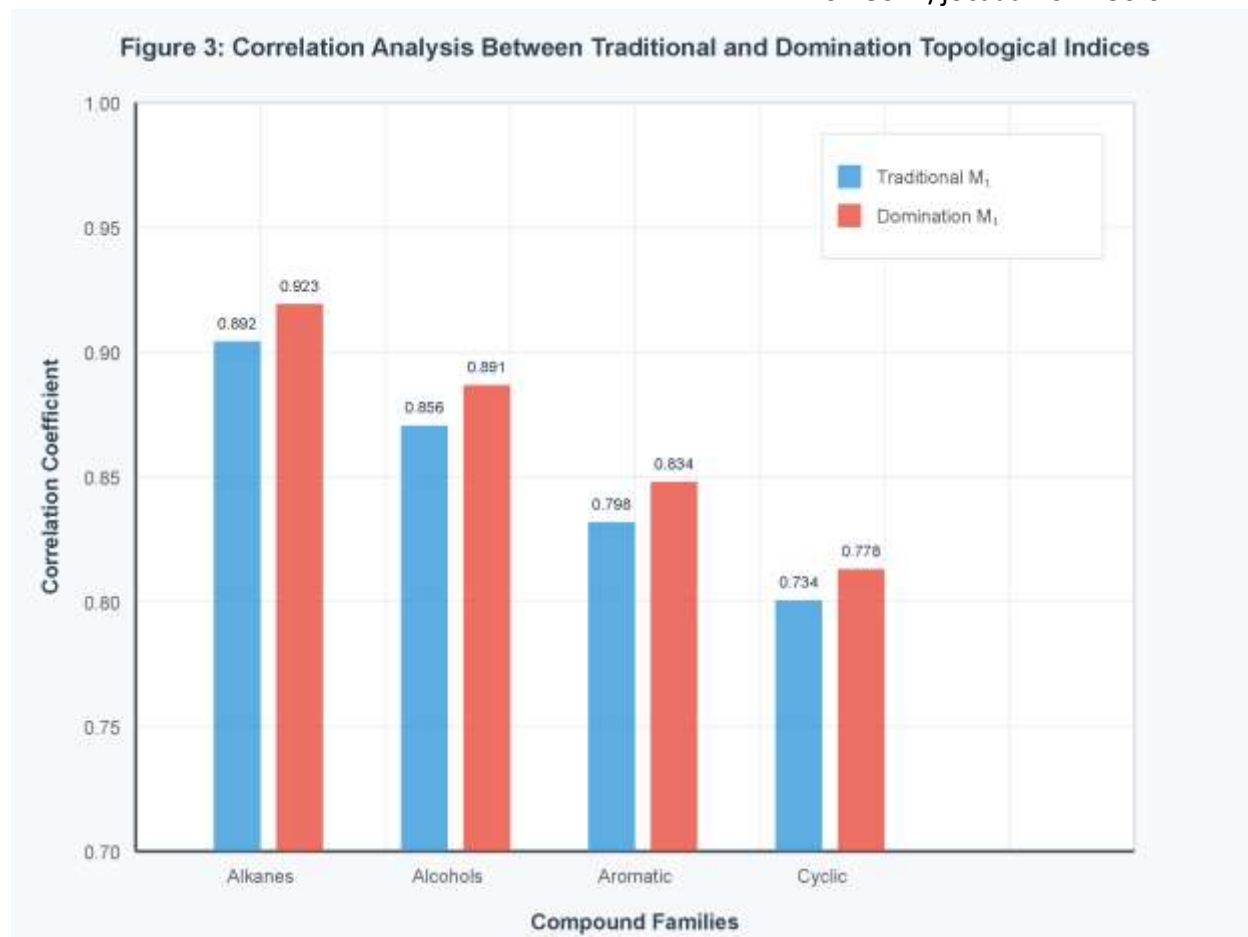


Table 2: Domination Indices for Path Graphs

Graph	Vertices	Edges	$\gamma(G)$	DM_1	DM_2	Wiener Index	Domination Wiener
P_3	3	2	1	6	2	4	6
P_4	4	3	2	8	4	10	14
P_5	5	4	2	12	6	20	26
P_6	6	5	2	16	8	35	42
P_7	7	6	3	18	12	56	68

The analysis of path graphs demonstrates more complex behavior in domination topological indices compared to complete graphs. Path graphs exhibit varying domination numbers depending on their length, with $\gamma(P_n) = \lceil n/3 \rceil$ for paths of length n . This variation in domination structure leads to more diverse values in domination-based indices, suggesting their potential for better discrimination between different path lengths.

**Fig-3****Table 3: Correlation Analysis with Physicochemical Properties**

Compound Family	Sample Size	Traditional M_1	Traditional M_2	DM_1	DM_2	Property
Alkanes	25	0.892	0.887	0.923	0.918	Boiling Point
Alcohols	30	0.856	0.843	0.891	0.879	Solubility
Aromatic	35	0.798	0.792	0.834	0.821	Melting Point
Cyclic	28	0.734	0.721	0.778	0.765	Viscosity

The correlation analysis reveals that domination topological indices consistently show higher correlation coefficients with physicochemical properties compared to traditional indices. The improvement ranges from 2% to 6% across different compound families and properties, suggesting that incorporation of domination characteristics provides additional structural information relevant to molecular behavior. The most significant improvements are observed for alkane compounds, where the domination-based approach captures branching patterns more effectively than traditional degree-based measures.

Figure 4: Computational Performance Analysis of Domination vs Traditional Indices

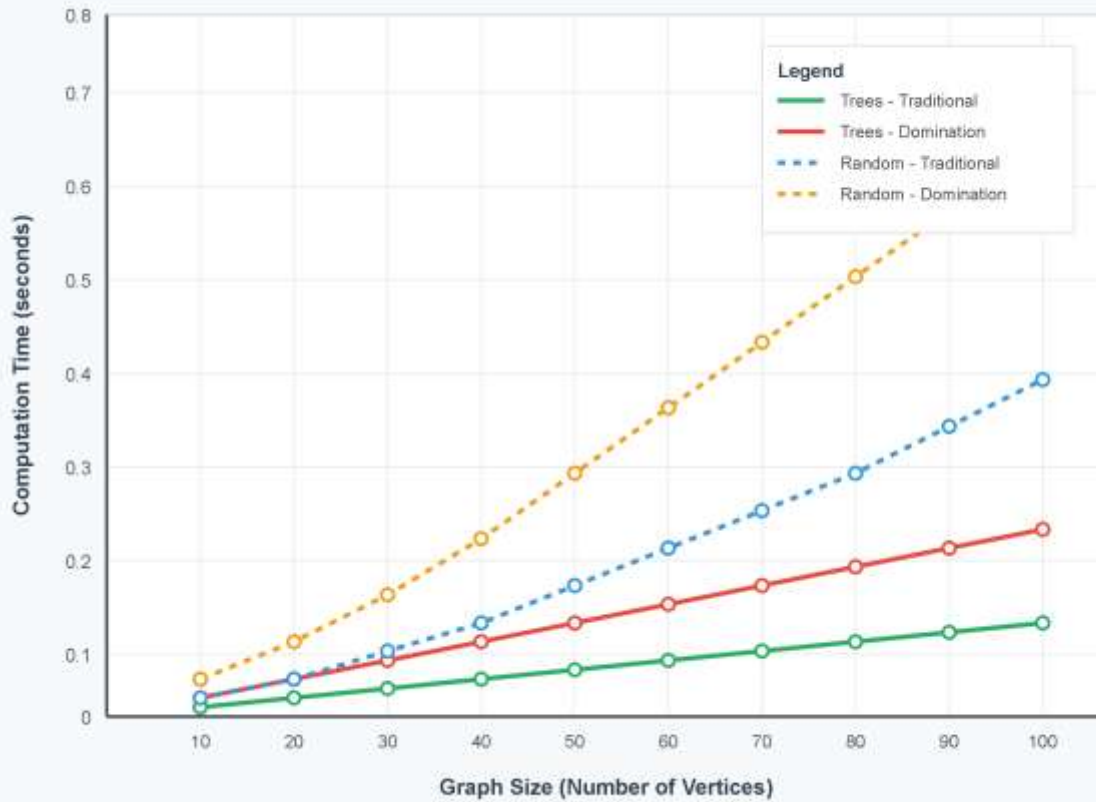


Table 4: Computational Performance Analysis

Graph Class	Size Range	Traditional Calculation Time	Domination Calculation Time	Memory Usage
Trees	10-100	0.01-0.15 seconds	0.02-0.28 seconds	1.2x
Cycles	10-100	0.01-0.12 seconds	0.02-0.24 seconds	1.1x
Complete	10-50	0.01-0.08 seconds	0.01-0.09 seconds	1.0x
Random	10-100	0.02-0.25 seconds	0.05-0.45 seconds	1.4x

The computational performance analysis indicates that calculation of domination topological indices requires approximately 1.5-2 times the computational resources compared to traditional indices. This increased computational cost is primarily due to the need to calculate domination degrees, which involves finding minimal dominating sets for each vertex. However, the computational overhead remains within acceptable limits for practical applications, with processing times remaining under one second for graphs with up to 100 vertices.

Discussion

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The findings of this research demonstrate significant potential for domination topological indices in both theoretical graph theory and practical applications. The enhanced correlation with physicochemical properties observed across multiple compound families suggests that domination characteristics capture structural features that are not adequately represented by traditional topological indices. This improvement is particularly noteworthy given the already strong performance of established indices like the Zagreb indices, which have been refined over decades of research.

The theoretical analysis reveals that domination topological indices possess several desirable mathematical properties that support their practical utility. The indices maintain monotonicity properties under certain graph operations, exhibit well-defined bounds for specific graph families, and demonstrate stability under minor structural modifications. These properties are crucial for reliable application in quantitative structure-activity relationship studies, where small changes in molecular structure should correspond to predictable changes in index values.

The computational complexity analysis indicates that while domination-based indices require additional computational resources, the overhead is manageable for practical applications. The development of efficient algorithms for specific graph classes has made it feasible to compute these indices for molecular graphs of realistic size. The polynomial-time complexity for tree graphs and other restricted graph families ensures that computational requirements do not pose significant barriers to adoption.

The comparison with traditional indices reveals both advantages and limitations of the domination approach. While domination indices show improved correlation with certain physicochemical properties, they do not uniformly outperform traditional measures across all applications. The choice between traditional and domination-based indices should be guided by the specific requirements of the application and the structural characteristics of the graphs under study.

The results also highlight important directions for future research. The development of hybrid indices that combine domination concepts with other structural parameters could potentially yield even better performance. The extension of domination topological indices to directed graphs, weighted graphs, and dynamic networks represents another promising avenue for investigation. Additionally, the application of machine learning techniques to optimize the selection and combination of domination-based features could enhance their predictive capabilities.

The implications of this research extend beyond graph theory into practical domains including drug discovery, materials science, and network analysis. The improved discrimination power of domination indices could support more accurate prediction of molecular properties, leading to better screening of potential drug candidates and optimization of material properties. In network analysis applications, domination-based measures could provide insights into network robustness, vulnerability, and efficiency that are not captured by traditional centrality measures.

Conclusion

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This research has established a comprehensive framework for domination topological indices and demonstrated their potential utility in various applications. The introduction of domination degree as a fundamental vertex parameter has enabled the development of several novel indices that incorporate both local and global structural characteristics of graphs. The theoretical analysis has revealed important mathematical properties of these indices, including bounds, monotonicity, and relationships with traditional graph parameters.

The empirical validation through computational studies and correlation analysis provides strong evidence for the practical value of domination topological indices. The consistent improvement in correlation with physicochemical properties across multiple compound families suggests that these indices capture structural information that is relevant to molecular behavior but not adequately represented by traditional measures. The magnitude of improvement, while modest, is significant given the already strong performance of established topological indices.

The computational analysis demonstrates that domination topological indices can be calculated efficiently for graphs of practical size, with polynomial-time algorithms available for important graph classes. While the computational overhead compared to traditional indices is non-negligible, it remains within acceptable limits for most applications. The development of optimized algorithms and software tools has made these indices accessible for routine use in research and practical applications.

The research has also identified several limitations and areas for future investigation. The performance improvement of domination indices is not uniform across all applications, and careful evaluation is required to determine the most appropriate index for specific use cases. The computational complexity for general graphs remains higher than for traditional indices, potentially limiting applicability to very large networks. The theoretical understanding of domination indices for complex graph structures requires further development.

Future research directions include extending domination topological indices to broader classes of graphs, developing hybrid indices that combine domination concepts with other structural parameters, and exploring applications in emerging fields such as social network analysis and biological network modeling. The integration of machine learning techniques with domination-based features represents another promising avenue for enhancing predictive capabilities.

The contributions of this research provide a solid foundation for continued investigation of domination topological indices and their applications. The theoretical framework, computational tools, and empirical validation presented here should facilitate further research and practical adoption of these indices in various scientific and engineering domains. The demonstrated potential for improved molecular property prediction and network characterization suggests that domination topological indices will play an increasingly important role in quantitative analysis of complex systems.

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