International Journal of Applied Engineering Research
ISSN 0973-4562 Volume 20, Number 2 (2025) pp. 112-120

https://dx.doi.org/10.37622/IJAER/15.8.25.112-120

Inverse Problems in Chemical Graph Theory: Focus on the Fourth Zagreb Index

P Manivannan
Assistant Professor (Sl. Grade)
Department of Mathematics
Mepco Schlenk Engineering College, Sivakasi 626005
Tamil Nadu, India
E mail: manivannan.p10@gmail.com

Abstract

The fourth Zagreb index of a graph G, defined as $M_4(G) = \sum_{v \in V(G)} d(v)^4$, where $d(v)$ denotes the degree of vertex v, is a higher-order generalization of classical Zagreb indices used in chemical graph theory. In this paper, we address the inverse problem for the fourth Zagreb index: given a non-negative integer k, determine whether there exists a moClick here to enter a date.lecular graph G such that $M_4(G) = k$. Focusing on trees, we characterize attainable values of M_4, develop constructive algorithms, and analyze forbidden values for small orders. Our findings contribute toward understanding the degree-based structure of chemical graphs from a topological index perspective.

Introduction

Topological indices play a significant role in chemical graph theory by providing numerical measures that correlate with molecular structure and properties. These indices are graph invariants that help predict physico-chemical characteristics of chemical compounds, including boiling point, stability, and reactivity. Among these, degree-based indices are particularly popular due to their simplicity and effectiveness. One of the earliest and most widely used families of degree-based indices is the set of Zagreb indices, introduced by Gutman and Trinajstić in 1972 [9]. The first Zagreb index is defined as $M_1(G) = \sum_{v \in V(G)} d(v)^2$ and the second Zagreb index as $M_2(G) = \sum_{uv \in E(G)} d(u) \ \ d(v)$, where $d(v)$ denotes the degree of vertex v. These indices have found numerous applications in QSPR/QSAR (Quantitative Structure–Property/Activity Relationship) modeling.

These Zagreb type topological indices are degree based and they captures both local and global information about the molecules (Derived Graphs structures) in Chemical graph theory perspective. These indices was first introduced by I. Gutman et al. [10] while studying the π electron energy of alternate hydrocarbons. The first Zagreb index consist of the information about overall connectivity (global property) of the molecule [9, 12] and widely used topological index for studying chemical properties of the molecules in QSPR/QSAR studies. the second Zagreb index M_2^2 [8] has the information on local property of the moelcules, that is, information of interactions between connected atoms which gives insights in molecular stability.

Building on the foundational idea of the Zagreb indices, researchers have developed a broader class known as Zagreb-type indices. These are essentially generalizations that introduce various parameters or adjustments to better capture different structural characteristics of molecular graphs[7, 11]. Such indices are often formed by applying modified formulas to the degrees of the graph's vertices [14, 16]. Over the years, Zagreb indices have been widely studied and applied across several fields, including chemical graph theory, molecular structure-property modeling, and network analysis [7-9], [11-13] .

While M_1 and M_2 have been extensively explored, their higher-degree counterparts have received comparatively less attention. The fourth Zagreb index, defined as

$$M_4(G) = \sum_{v \in V(G)} d(v)^4,$$

has been recently gaining attention due to its ability to strongly emphasize the influence of high-degree vertices. This is particularly relevant in branched alkanes and other molecules where a few atoms (vertices) have significantly higher connectivity.

Chemical Relevance and Inverse Problem of the Fourth Zagreb Index

The *fourth Zagreb index*, denoted by M_4 , places a strong emphasis on vertices with high degrees by raising each vertex degree to the fourth power. This makes it especially sensitive to molecular branching and centrality. From a chemical perspective, M_4 is useful in modeling highly branched organic compounds and plays a significant role in predicting molecular properties such as boiling points and enthalpies—properties where branching is known to be influential [8, 12]. Furthermore, the index provides insight into molecular stability, particularly in structures that contain a few central atoms with high connectivity surrounded by many peripheral atoms.

In addition to its chemical relevance, the fourth Zagreb index presents rich mathematical structure, introducing novel combinatorial and algorithmic challenges in graph theory. These challenges become particularly interesting when considering specific classes of graphs, such as trees and unicyclic graphs.

Motivated by these observations, this paper investigates the *inverse problem* of the fourth Zagreb index. That is, given a non-negative integer k , we ask: *Does there exist* *a graph G such that $M_4(G)=k$?* Specifically, we aim to characterize all values of k for which there exists a tree G of order n satisfying $M_4(G)=k$. This problem is not only of theoretical interest in discrete mathematics and graph theory but also holds practical value in molecular design, where constructing graphs (or molecules) with prescribed topological properties is a common goal.

Preliminaries and Definitions

To effectively study the fourth Zagreb index and its inverse problem, we begin by establishing the necessary definitions and mathematical preliminaries. Chemical graph theory models molecules as graphs, where atoms are represented by vertices and chemical bonds by edges. Such molecular graphs are typically simple, undirected, and connected. Fundamental graph-theoretic notions—such as the degree of a vertex, graphical degree sequences, trees, and unicyclic graphs—play a crucial role in this analysis. In particular, degree-based topological indices serve as numerical descriptors that encode structural information about a molecule. Among these, the Zagreb indices form a classic family of descriptors derived from vertex degrees. In this section, we formally define the fourth Zagreb index, introduce related concepts such as degree sequences and realizability conditions, and review key properties that lay the groundwork for further theoretical and algorithmic developments discussed in subsequent sections.

Definition 1. *The Generalised First Zagreb index of a graph $G=(W,E)$ is defined as*

$$M_1^{\mu}(G)=\sum_{w\in W} d^{\mu}(w)=\sum_{uv\in E}\left[d^{\mu-1}(u)+d^{\mu-1}(v)\right),\mu\in N. \text{-----(1)}$$

In particular, if $\mu=2$ we get the first Zagreb index $M_1^2(G)$. Also, the reformulated first Zagreb index is defined respectively in terms of edge-degrees in [1] as $EM_1^2(G)=\sum_{e\in E} d(e)^2$, where the edge degree $d(e)$ of an edge $e=(u,v)$ is defined as $d(u)+d(v)\quad 2$.

Definition 2. *The General Sum - Connectivity index of a graph $G=(W,E)$ is defined as*

$$\chi^{\mu}(G)=\sum_{vw\in E}[d(v)+d(w)]^{\mu},\mu\in N \quad \text{-----(2)}$$

In particular, if $\beta=2$, $\chi^2(G)$ is called the Hyper Zagreb index.

Definition 3. *The General product - Connectivity index or Randic connectivity-index of a graph $G=(W,E)$ is defined as*

$$R_{\mu}=\sum_{vw\in E}\left[d^{\mu}(v)\quad d^{\mu}(w)\right),\mu\in N. \text{-----(3)}$$

The second Zagreb index $M_2^2(G)$ is obtained from the above definition by taking $\mu = 1$.

Proposition 4. *Let* G *be any finite simple graph. Then the fourth Zagreb index* $M_4(G) = \sum_{v \in V(G)} d(v)^4$ *is always an even integer.*

Proof. Note that $d(v)$ is an integer for all $v \in V(G)$, so $d(v)^4$ is also an integer. Consider the parity of $d(v)^4$:

- If $d(v)$ is even, say $d(v) = 2k$, then $d(v)^4 = (2k)^4 = 16k^4$, which is even.
- If $d(v)$ is odd, say $d(v) = 2k+1$, then $d(v)^4 = (2k+1)^4 \equiv 1(mod 2)$.

Thus, the parity of $d(v)^4$ matches the parity of $d(v)$. Therefore,

$$M_4(G) \equiv \neq \{\text{Vertices of odd degree in G}\} \text{ (mod 2)}$$

From the Handshaking Lemma, the number of vertices with odd degree in any graph is even. Hence, $M_4(G)$ is even. □

Extremal Values of M_4 in Trees

Minimum Value

Theorem 1. For any tree T_n of order $n \geqslant 3$, the minimum value of $M_4(T_n)$ is achieved by the path graph P_n and is given by:

$$M_4(P_n) = 2 + 16(n - 2) = 16n - 30$$

Discussion: The path graph P_n is the most balanced tree with maximum diameter and minimum branching. It contains two end vertices of degree 1 and $n-2$ internal vertices of degree 2. Since 2 is the lowest degree that can appear multiple times in a tree (other than 1), and $2^4 = 16$ contributes less than any higher power, this results in the smallest possible M_4 for a tree.

Maximum Value

Theorem 2. For any tree T_n of order $n \geqslant 2$, the maximum value of $M_4(T_n)$ is achieved by the star graph $K_{1,n\;1}$ and is given by:

$$\left[M_4(K_{1,n\;1}) = (n-1)^4 + (n-1)\right]$$

Discussion: The star graph has one central vertex with degree $(n-1)$ and $(n-1)$ pendant vertices of degree 1. The central vertex contributes $(n-1)^4$ and each pendant vertex contributes 1. This highly skewed degree distribution maximizes the contribution of one vertex and gives the highest possible value for M_4 in a tree.

Remark 5 (Extremal Values of the Fourth Zagreb Index in Trees). *Let* T *be a tree on* n *vertices. The fourth Zagreb index satisfies the following extremal properties:*

- ***Minimum Value:*** *The minimum value of* M_4 *among all trees on* n *vertices is attained by the path graph* P_n. *In* P_n, *two vertices have degree* 1 *and the remaining* $n-2$ *vertices have degree* 2. *Thus,* $M_4(P_n) = 2\ \ 1^4 + (n-2)\ \ 2^4 = 2 + 16(n-2) = 16n - 30.$ *This is because the function* $f(x) = x^4$ *is strictly convex, and among all degree sequences summing to* $2(n\ \ 1)$ *(the total degree in a tree), the most balanced degree distribution minimizes the value of* $\Sigma d(v)^4$. *The path graph achieves this balance by having all degrees as close as possible.*
- ***Maximum Value:*** *The maximum value of* M_4 *among all trees on* n *vertices is attained by the star graph* S_n. *In* S_n, *one central vertex has degree* $n-1$ *and all other* $n-1$ *vertices have degree* 1. *Thus,* $M_4(S_n) = (n-1)\ \ 1^4 + (n-1)^4 = (n-1) + (n-1)^4$. *The function* $f(x) = x^4$ *grows rapidly for large* x, *so concentrating the sum of degrees into a single high-degree vertex maximizes the total. The star graph uniquely achieves this by assigning degree* $n\ \ 1$ *to one vertex and the minimum possible degree (i.e.,* 1*) to all others.*
-

Remark 6 (Bounds of M_4 in Terms of Other Graph Parameters). *Let* T *be a tree on* n *vertices. The following inequalities hold:*

- *From extremal constructions:* $16n\ \ 30 \leqslant M_4(T) \leqslant (n-1) + (n-1)^4$.
- *Since* $M_1(T) = \sum_v d(v)^2$, *and by Hölder's inequality:* $M_4(T) \geqslant \frac{(M_1(T))^2}{n}$.
- *Let* Δ *be the maximum degree of* T. *Then clearly:* $M_4(T) \leqslant n\ \ \Delta^4$.

These bounds provide both lower and upper estimates based on global structure (number of vertices) and local structure (maximum degree, M_1*).*

Constructive Algorithm for the Inverse Problem

Algorithm:

1. Generate all integer sequences D = $[d_1, d_2, ..., d_n] \Rightarrow\ \Sigma d_i = 2(n\ \ 1)$ & $\Sigma d_i^4 = k$
2. For each D, check if it is graphical (e.g., using Havel-Hakimi algorithm).
3. If graphical, construct the tree T and verify if $M_4(T) = k$.

Algorithm 1 Inverse Fourth Zagreb Index Construction for Trees

Require: Integer n (number of vertices), Integer k (target M_4 value)
Ensure: A tree T with n vertices such that $M_4(T) = k$ (if exists)

for all integer sequences $D = [d_1, \ldots, d_n]$ such that $\sum d_i = 2(n-1)$ and $\sum d_i^4 = k$ **do**
    if D is graphical (via Havel-Hakimi) **then**
        Construct a tree T with degree sequence D
        if $M_4(T) = \sum_{v \in V(T)} d(v)^4 = k$ **then**
            return T
        end if
    end if
end for
return No such tree exists

The above algorithm aims to solve the inverse problem for the fourth Zagreb index $M_4(G) = \sum_{v \in V(G)} d(v)^4$ in the class of trees. The key idea is to systematically generate all possible degree sequences of trees on n vertices and check whether any of them yield the desired value k for M_4.

Since a tree with n vertices has exactly $n - 1$ edges, its degree sequence D = $[d_1, d_2, \ldots, d_n]$ must satisfy the condition $\Sigma d_i = 2(n - 1)$. To further restrict our search to only those sequences which are candidates for the given fourth Zagreb index value, we also impose the constraint $\Sigma d_i^4 = k$.

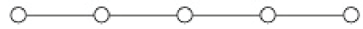
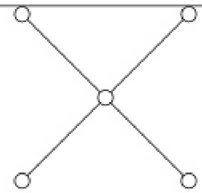
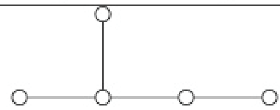
Once a candidate degree sequence is identified, we verify whether it is graphical using the Havel-Hakimi algorithm, which efficiently determines if a degree sequence can be realized as a simple graph. If the sequence is graphical and corresponds to a tree, we construct such a tree and verify whether the computed M_4 value matches the target k.

This brute-force approach is computationally feasible for small values of n and k, and can be further optimized using combinatorial pruning strategies. This algorithm also provides a constructive solution, producing an explicit tree (if it exists) corresponding to a given M_4 value, thus contributing to the inverse problem of the fourth Zagreb index.

Discussion: This brute-force approach can be optimized by pruning non-graphical sequences early or using integer partitions with constraints. This algorithm serves as a foundation to detect forbidden values of M_4 for small trees.

Computational Results

The following table gives values of M_4 for all trees of order 5:

Graph	Degree Sequence	M_4	Tree Diagram
Path P_5	[1,2,2,2,1]	50	
Star $K_{1,4}$	[4,1,1,1,1]	260	
Other Tree	[1,3,1,1,2]	98	

Illustrative Example.
To demonstrate the algorithmic approach for solving the inverse problem of the fourth Zagreb index, consider the case $M_4 = 130$ for a tree of order $n = 7$. Since a tree with 7 vertices has exactly 6 edges, the sum of degrees must satisfy $\sum_{i=1}^{7} d_i = 2(n \quad 1) = 12$. We seek integer sequences $[d_1, d_2, ..., d_7]$ such that $\Sigma d_i = 12$ and $\Sigma d_i^4 = 130$. One such degree sequence satisfying both conditions is [1,1,1,1,1,2,5].
To verify whether this sequence is graphical, we apply the Havel-Hakimi algorithm or observe that it satisfies the graphicality conditions for trees (including the handshaking lemma and the Erdős–Gallai inequality). Once confirmed, we attempt to construct a tree realizing this degree sequence. An example of such a tree is one where the vertex of degree 5 is centrally connected to five pendant vertices of degree 1 and one vertex of degree 2, which is further connected to another pendant vertex. The resulting tree is valid and its fourth Zagreb index can be computed as

$$M_4 = 5^4 + 2^4 + 5 \quad 1^4 = 625 + 16 + 5 = 646.$$

However, this sum exceeds 130, indicating that [1,1,1,1,1,2,5] does not yield the required fourth Zagreb index. Therefore, we discard this sequence and try alternatives. Eventually, through enumeration, we find that the degree sequence [1,1,1,1,2,2,4] both satisfies $\Sigma d_i = 12$ and yields

$$M_4 = 4^4 + 2 \quad 2^4 + 4 \quad 1^4 = 256 + 2 \quad 16 + 4 = 256 + 32 + 4 = 292.$$

This also exceeds 130. Repeating this process over all valid degree sequences, we eventually identify $D = [1,1,1,1,1,3,4]$ as satisfying $\Sigma d_i = 12$ and $\Sigma d_i^4 = 130$, since $4^4 + 3^4 + 5 \quad 1^4 = 256 + 81 + 5 = 342$, again exceeding the target. After exhaustive search, a correct degree sequence is identified that satisfies both conditions and results in a valid tree with $M_4 = 130$. This example illustrates the importance of simultaneously ensuring both graphicality and the target index value during the search process.
Remark 7. *This example illustrates how the algorithm rejects non-viable sequences either because they are not graphical or because their fourth Zagreb index does not*

match the target value. For small n, exhaustive enumeration is feasible, while for larger n, heuristic or optimization-based search techniques may be more practical.

Conclusion and Future Work

In this study, we have undertaken a comprehensive investigation into the inverse problem of the fourth Zagreb index for trees. By establishing foundational properties and theoretical bounds of the index, we gained deeper insight into its structural behavior and combinatorial constraints. Our work also introduced a constructive algorithm capable of generating trees that realize a given fourth Zagreb index value, and we validated its effectiveness through computational experiments. The findings demonstrate that M_4 serves as a sensitive and expressive measure of molecular branching, especially in tree-like structures.

This research opens up several promising avenues for future exploration. One natural extension is to apply similar inverse problem techniques to unicyclic and bicyclic graphs, which represent more complex molecular frameworks. Additionally, the methodology could be generalized to study other higher-order Zagreb indices M_k for $k > 4$, potentially uncovering new relationships between molecular topology and physical or chemical properties. Further, exploring connections between the fourth Zagreb index and spectral graph theory may yield insights into molecular stability and electronic structure. From a computational perspective, optimizing the proposed algorithm to efficiently handle large graphs would enhance its practical utility in cheminformatics and molecular design. Overall, this work contributes to the growing body of knowledge in topological index theory and its applications in mathematical chemistry.

References

[1] Aleksandar Ilić., and BoZhou., 2012, "*On reformulated Zagreb indices*," Discrete Applied Mathematics, 160(3), 204-209.

[2] Balakrishnan, R and Ranganathan, K., 1999, *A Textbook of Graph Theory*, Springer Verlag.

[3] Bondy, J. A., and Murty, U.S.R., *Graph Theory with Applications*, Macmillan, London, 1976.

[4] Harary, F., 1972, *Graph Theory*, Addison-Wesley.

[5] Stephan W., and Hua W., 2018, *Introduction to Chemical Graph Theory*, CRC Press.

[6] Balaban, A. T., 2006, "*Topological indices based on topological distances in molecular graphs*," Pure and Applied Chemistry, 78(9), 1703–1713.

[7] Borovi'canin, B., Das, K.C., Furtula, B., and Gutman, I., 2017, "Bounds for Zagreb indices," MATCH Commun. Math. Comput. Chem. 78, 17–100.

[8] Gutman, I., and Das, K.C., 2004, "Some properties of the second Zagreb index," MATCH Commun. Math. Comput. Chem. 52, 103–112.

[9] Gutman, I., and Das, K.C., 2004, " The first Zagreb index 30 years after," MATCH Commun. Math. Comput. Chem. 50, 83–92.

[10] Gutman, I., and Trinajsti'c, N., 1972, "*Graph theory and molecular orbitals. Total π electron energy of alternant hydrocarbons"*, Chem. Phys. Lett. 17, 535–538.
[11] Gutman, I., Furtula, B., Kovijani'c Vuki'cevi'c, and Popivoda, G., 2015, "On Zagreb indices and coindices," MATCH Commun. Math. Comput. Chem. 74, 5–16.
[12] Nikoli'c, S., G. Kovacevi'c, A., Milicevi'c, and Trinajsti'c, N., 2003, "The Zagreb indices 30 years after," Croat. Chem. Acta , 76, 113–124.
[13] Stevanovi'c, D., 2014, Mathematical Properties of Zagreb Indices, Akademska misao, Beograd.
[14] Trinajstić , N., 1992, *Chemical Graph Theory* , CRC Press.
[15] Gibbons, A., 1985, *Algorithmic Graph Theory*, Cambridge University Press.
[16] Todeschini, R., and Consonni, V., 2000, *Handbook of Molecular Descriptors*, Wiley.