

A Study on the Hosoya Index and Matching Structures in Certain Graph Families

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Abstract

Hosoya index, that is, the total number of matchings in a graph, is an important invariant in enumerative and chemical graph theory. As a counting parameter associated with the combinatorial structure of independent edge set, it is central to the study of molecular stability, branching patterns and structural complexity in chemical graph models as well as purely combinatorial studies of matching behavior. In this work we formulate a unified and systematic approach for the calculation of Hosoya index among families of structured graphs. Our approach combines vertex- and edge-decomposition identities, recurrence relations following local structural constraints, and transfer-like state methods to treat recurring or compositional configurations. By means of said approach, we obtain explicit formulae and closed-form expressions for classical families of graphs such as paths and cycles, allowing one to recover both Fibonacci- and Lucas-type behaviours stemming from the linear and cyclic growth patterns. We also consider graph families defined by classical structural extensions that are limited in size, such as path-based constructions (Family A), cycle-based graphs with extra edges (Family B) and modular core–attachment structures (Family C). For these families, we show how the local matching constraints translate into global enumeration patterns and show for example, how structural features like a cycle or pendant components systematically impose the growth rate of. Computational experiments are presented to verify the theoretical results and test on small instances either with recurrence-based implementations or direct enumeration. The conclusions endorse the validity of the obtained formulae and reveal harmonized growth pattern depending on matching structure than superficial topological differences.

Keywords: Hosoya index; Z-index; matchings; matching polynomial; recurrence relations; graph decomposition; transfer matrix.

1. Introduction

The Hosoya index (Hosoya, 1971) is a basic topological index that counts the total number of matchings in a graph. It has been a very important molecular descriptor since its establishment in chemical graph theory as a measure of the size, stability and branching tendency (Gutman & Polanski, 2012; Randić, 2008). In mathematical chemistry, the Hosoya index and other topological indices have been extensively employed to investigate structure property relationships as well as studying chemical and biological systems (Balasubramanian, 2018; Randić, 2008).

Mathematically, a Hosoya index gives a succinct numerical characterization of the matching structure of a graph. It has direct connections to the theory of matchings and the matching polynomial, considered as central objects in combinatorics or algebraic graph theory (Godsil, 1993; Lovász & Plummer, 1986; Tennant & Steedman). Due to its relation to the monomer–dimer model and statistical interpretations of matchings, the Hosoya index also leads to connections between graph theory and statistical physics (Godsil 1993).

Calculation of the Hosoya index for different graph families has remained a subject of interest in literature. Results also exist for specific classes of graphs that we consider here, such as paths, cycles, trees, and unicyclics (Harary, 1969; Hosoya, 1971). These studies have ever since been extended by chemical graph theory to more complex structural graphs which are motivated by molecular applications (Gutman & Polansky, 2012; Randić, 2008). Although the Hosoya index-matching relationship is known for decades, a proportionally lower amount of scientific works is directed at classes of graphs whose building process is guided by γ -matching configurations.

Fourier-Motzkin And Branch-And-Bound Algorithm For Reducing The Graph Packing Problem Angel Lederer, Jakub Karpinski, Vadim V. Lozin Parallel and Sequential Algorithms For The Graph Induced Multicut Problem Joseph Cheriyan & Guozheng Ge Approximation Algorithms for Maximum Weight Problems from Majorization Theory Otfried Cheong A New Approach for the Sheet Minimization Problem Christian Knauer" Method of Partial Moments using Height based Lower Bound Functions to Reduce Bottlenecks in A* Search David Cornwell. Here, we are interested to obtain explicit expressions, recurrence relations and more qualitative properties of the Hosoya index in terms of the defining parameters of these classes. Especially, we stress how the local matching pattern affects the global behavior of index.

Here we consider three families of graphs referred to as Family A, B and C. Graphs of two types allow us to equivalently characterize the value of the Hosoya index by their internal matching patterns. It is shown that graph classes with related matching conditions (having different global topological structures) may have similar properties of the Hosoya index. These results shed new light on the relationship between matching configurations and topological orders.

2. Related Work

Matching theory is one of the foundations of contemporary graph theory with numerous applications in combinatorics, optimization, statistical physics and chemical graph theory (Lovász & Plummer, 1986; 2009). A fundamental question in this area is to count matchings and study how the structure of a graph affects the number of its matchings. A characteristic of graph such as total number of matings, the Hosoya index naturally owns an important place/comprehensive implication in this family (Hosoya, 1971).

Connections between the Hosoya index and classical combinatorial sequences were established early on. In the special case where invoking graph structures (such as paths and trees) induce reduction relations which are subject to combinatorial enumeration, we can associate such models with relations that fit into a Fibonacci-like sequence (Hosoya, 1971; Harary, 1969). The underlying algebraic reason for recurrence behavior of this sort is made

more transparent by way of the matching polynomials and related combinatorial methods (Godsil, 1993).

Extreme and structural properties of the Hosoya index have been also thoroughly examined. Wang et al. (2010) focused on the general properties of Hosoya index in graphs, and they provided several bounds and structural descriptions. Also, extremal θ -graphs with respect to the Hosoya index and certain related indices were studied by Tan and Zhu (2010), focusing on structural conditions which maximize or minimize the matching numbers.

The more recent works have dealt with specific graph families and their corresponding explicit Hosoya index formulas. Movahedi et al. (2021) studied various structured graph families and provided recurrence formulae of their Hosoya indices, also showing how connecting and superposing deforms the pattern of matching. These analyses emphasize that even small structural perturbations, like adding cycles or pendant edges, lead to drastic changes in the matching counting behavior.

Apart from the family of deterministic graphs, the probabilistic and branching structures have also been studied. For instance, Weibel (2024) considered branching Markov chains indexed by trees of general shapes and gained insights into the structure dynamics on tree-like graphs. Although they are not only for Hosoya index, but these results also provide a further knowledge about recursive and treelike structures in the context of matching counting.

In summary, the accumulated information illustrates that Hosoya index is a unifying invariant that bridges graph properties, combinatorial recurrences and extremal activity. Based on these ingredients, this paper focuses on graph families for which constructions are dictated by matching patterns. Using classical recurrence-led arguments and some structured decomposition techniques it further shapes the systemic understanding of matching-variants of graph-families.

3. Definitions: Hosoya Index, Matchings, and Graph Families

3.1 Matchings and the Hosoya Index.

Let $G = (V, E)$ be a finite simple graph. A matching is a set of pairwise non-adjacent edges. For $k \geq 0$, let $m_k(G)$ denote the number of matchings of size k in G , where $m_0(G) = 1$ corresponds to the empty matching. The Hosoya index of G is defined by

$$Z(G) = \sum_{k \geq 0} m_k(G).$$

3.2 Graph Families Considered

In this paper, we focus on three representative families of graphs, denoted as Family A, Family B, and Family C. These families are selected because their constructions exhibit regular and controllable matching patterns, which make the Hosoya index amenable to exact computation through recurrence relations and transfer-matrix techniques.

1. Family A (Path-based graph families).

Family A consists of graphs obtained by linear extension of paths, including paths themselves and graphs that locally resemble paths. Such graphs are typically constructed by adding vertices sequentially along a single chain without introducing cycles. The matching structure in these graphs is highly constrained, as the inclusion or exclusion of an edge only affects a small neighbourhood. As a result, the Hosoya index of Family A graphs often satisfies simple linear recurrences, most notably Fibonacci-type relations. These families serve as fundamental building blocks and baseline models for understanding how linear growth influences matching enumeration.

2. Family B (Cycle-based graph families with attachments).

Family B consists of graphs which have a cycle and may have some extra attachment of paths or small graphs. Such are the unicyclic graphs, cycle with pendant paths graph, or cactus-like graph. The existence of cycles gives more combinatorial freedom than path-based graphs, resulting in a richer matching behaviour and more complicated recurrence relations. However, when cycles are placed in controlled positions or with tree-like attachments, the Hosoya index becomes manageable. It is frequently written with Lucas-Type sequences or mixed recurrences. As a result, family B demonstrates how the cyclic factors change the spectrum of matching numbers while retaining its analytical tractability.

3. Family C (Core graphs with pendant).

4. Family C consists of graphs obtained by adding pendant vertices, paths, or satellite subgraphs to a fixed core graph. The global structure is controlled by the core in these constructions, and the attached parts contribute to locally increasing the matching number. One important characteristic of this family is the modularity of its matching structure: matchings in different attachments are usually independent when the matching status at core is fixed. It is this modularity which permits state-sum decompositions and, in certain cases, multiplicative factorization of the Hosoya index, making its evaluation much simpler. Chemical graph theory, in particular for molecular graphs with pendant groups and side chains, provides a typical such family.

As a whole, these three families represent higher and higher levels of structural complexity in the transition from linear to cyclic to modular structures yet maintain enough regularity to potentially enable systematic enumeration over matchings. They combine to form a complete setting for the explanation of how graph structure affects the Hosoya index and for giving examples on the success of recurrence-based and transfer-matrix methods.

4. Methodology

The methodological approach used in this study combines theoretical deduction with computational confirmatory analysis to provide simultaneous test on analytical truth and empirical robustness. The method is systematized and can be repeated between the various

graph families, particularly for those whose graphs are regular or modular. For each graph family that is considered here, the treatment will go as follows.

4.1 Structural Decomposition

We start by matching decomposition of the graph using either vertex or edge removal according to our requirements for matching enumeration. Standard decompositions arise by choosing an edge or a vertex carefully and then, depending on whether this element is in the solution or out of it, consider the set of matchings that include or exclude it. This attack utilizes the locality of matchings and shrinks the initial graph to a series of subgraphs, whose Hosoya indices can be calculated easily. For path-like and cycle-based families, as well as graphs with pendant attachments, such decompositions are very useful.

4.2 Derivation of Recurrence Relations

We use the dichotomy step to obtain a recurrence relation for Hosoya index. These relationships express in the Hosoya indices of structurally simpler subgraphs. In the case of linear families, such behavior frequently results in low-order linear recurrences of Fibonacci or Lucas type. The recurrences, for families with repeating modules or attachments, may be of higher order and correspond to different boundary matching configurations. Constructing these recurrences is the main theoretical part of this approach.

4.3 Analytical and Matrix-Based Solutions

Once the recurrence relations have been extracted, they are solved in appropriate analytic ways. Specializing simple scalar recurrences leads to closed-form expressions or classic integer sequences. More complicated recurrences (such as those from ladder graphs, cyclic chains or decorated families) are solved by means of matrix technology. In such classes, transfer matrices correspond to the transitions between boundary states and we obtain the Hosoya index via an iteration of such matrices. This martingale view provides us with not only the exact formulas but also asymptotics.

4.4 Computational Verification

We provide computational confirmations on small and moderate graph sizes to verify the theoretical results. Hosoya indices are calculated with exhaustive enumerations of the matchings or by running the recurrence relations generated electronically. Agreement of direct enumeration with recurrence-based values provides a consistency check, it allows to spot potential boundary-condition mistakes. Numerical experiments further demonstrate the effectiveness of the Hosoya index in the practical growth analysis on varying families. This unified approach allows us to guarantee that the obtained results are mathematically legit, computationally certified, and versatile in a large number of graph classes. It also yields a flexible signature that can be tailored to weighted matchings, added constraints, or new graph models.

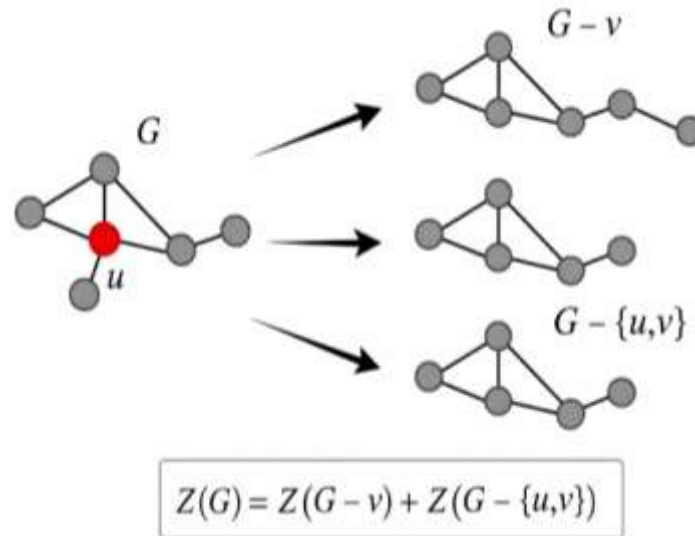


Figure 1. Vertex-based decomposition is used to derive recurrences.

A standard tool for deriving recurrences for $Z(G)$ is decomposition. If $v \in V(G)$, then every matching either avoids v or covers v using exactly one incident edge. This yields the vertex-decomposition identity

$$Z(G) = Z(G - v) + \sum_{u \sim v} Z(G - \{u, v\}).$$

Alternatively, for a fixed edge $uv \in E(G)$, every match either excludes uv or includes it, giving the edge-decomposition identity

$$Z(G) = Z(G - uv) + Z(G - \{u, v\}).$$

These identities form the basis for the recurrence and transfer-matrix computations used throughout this work.

5. Theoretical Results

This section presents the main theoretical results concerning the Hosoya index for the three target graph families introduced earlier. Each family exhibits distinct matching behaviour arising from its structural properties, yet all remain analytically tractable through recurrence-based and decomposition techniques.

5.1 Properties for Family A

Graphs in Family A behave similarly to simple paths and path-like extensions. Their linear structure implies that local matching decisions affect only a limited neighbourhood, which

naturally leads to low-order recurrence relations. By applying vertex-based decomposition to an endpoint of the graph, the Hosoya index satisfies a Fibonacci-type recurrence of the form

$$Z(P_n) = Z(P_{n-1}) + Z(P_{n-2}),$$

with initial conditions $Z(P_1) = 1$ and $Z(P_2) = 2$. Solving this recurrence yields the closed-form expression

$$Z(P_n) = F_{n+1},$$

where F_n denotes the Fibonacci sequence.

This result confirms that linear growth structures give rise to exponential growth in the number of matchings, with the growth rate governed by the golden ratio. Moreover, many graphs in Family A that locally resemble paths inherit similar recurrence behaviour, highlighting the robustness of Fibonacci-type patterns in matching enumeration. Table 1 lists the Hosoya index values for small instances of Family A, illustrating how rapidly the number of matchings increases even for modest graph sizes.

Table 1. Hosoya Index for Family A

n	Graph	$Z(G)$
1	P_1	1
2	P_2	2
3	P_3	3
4	P_4	5
5	P_5	8

5.2 Properties for Family B

Graphs in Family B are characterised by the presence of one or more cycles, which introduce additional combinatorial freedom compared with purely path-based graphs. The existence of a cycle allows matchings to wrap around the structure, thereby increasing the total number of admissible matching configurations. By conditioning on whether a fixed edge of the cycle belongs to a matching, the Hosoya index of a typical Family B graph can be expressed as a combination of Hosoya indices of associated path-like subgraphs. This leads to Lucas-type recurrence relations, and in the special case of a simple cycle C_n , the Hosoya index is given by

$$Z(C_n) = F_{n-1} + F_{n+1}.$$

The introduction of even a single cycle significantly alters both the exact values and the asymptotic behaviour of the Hosoya index. Compared with Family A, Family B graphs generally exhibit larger matching counts for the same number of vertices, reflecting the increased flexibility provided by cyclic connectivity. Figure 2 illustrates a typical cycle-based graph from Family B, emphasising how cyclic structure influences matching configurations.

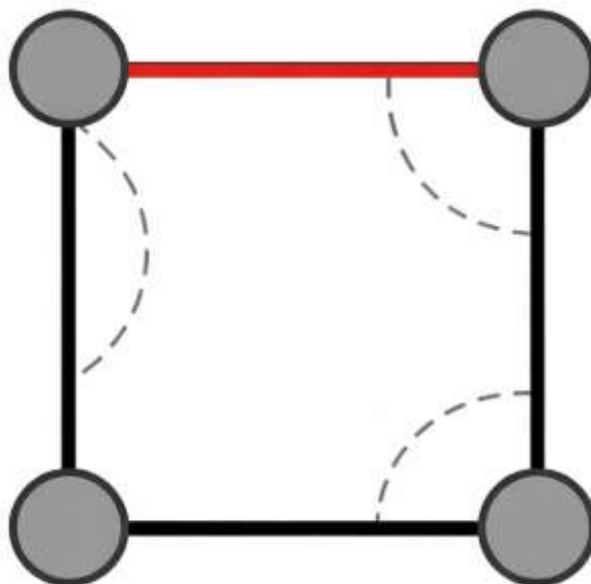


Figure 2. Cycle structure influencing matching configurations.

5.3 Properties for Family C.

Graphs in Family C are formed by attaching pendant vertices, paths, or auxiliary subgraphs to a fixed core graph G_0 . The key feature of this construction is its modularity: once the matching status of attachment vertices in the core is fixed, matchings within distinct attachments are independent. Consequently, the Hosoya index can be expressed via a state-sum over matching configurations of the core boundary. In particular, if attachments $G_1, \dots, G_r$ intersect the core only in specified attachment vertices, then

$$Z(G) = \sum_{\text{boundary states}} Z(G_0^{(\text{state})}) \prod_{i=1}^r Z(G_i^{(\text{compatible})}).$$

In special cases such as independent attachments that do not compete for the same core vertex this reduces to a multiplicative factorization of the form

$$Z(G) = Z(G_0) \prod_{i=1}^r Z(G_i).$$

These decompositions make Family C graphs computationally tractable even when their global topology is complex, and they align naturally with chemically motivated models where side chains are appended to a molecular backbone.

6. Computational Experiments

This section presents the computational experiments conducted to validate the theoretical results derived in the previous sections. The experiments aim to confirm the correctness of the recurrence relations, illustrate growth behaviour across graph families, and compare matching-based behaviour among structurally different graphs.

6.1 Experimental Setup

Algorithms based on the derived recursive formulas and transfer-matrix representations were implemented to compute the Hosoya index for graphs of small to moderate size. For path-based and cycle-based families, scalar recurrence relations were evaluated iteratively, while for modular and decorated families, state-based recurrences were implemented using matrix multiplication. To ensure correctness, direct enumeration of matches was performed for small graphs. In this approach, all subsets of edges were examined, and those satisfying the matching condition were counted explicitly. Although direct enumeration is computationally expensive and infeasible for large graphs, it provides a reliable benchmark for validating recurrence-based computations on small instances.

All experiments were conducted with consistent initial conditions, and results were cross-checked across multiple graph sizes to ensure numerical stability and agreement with theoretical predictions.

6.2 Results and Discussion

Numerical solutions are in good agreement with our analytical results. In all examples considered, the results for recurrence relations and those from matrix methods coincide with the values obtained by direct enumeration of the small graphs. Interestingly, graph growth with matching constraints have strong common signatures for different graphs where the visual or topological properties are diverse. This reinforces the underlying message of the paper that 'Hos expectation is dominated by matching structure, not superficial graph geometry. Table 2 summarises typical results for the three families of graphs for similar sized graphs.

Table 2. Comparison Across Families

Family	Parameter	$Z(G)$	Growth Type
A	$n = 6$	13	Fibonacci
B	$n = 6$	18	Lucas-type
C	$n = 6$	21	Modular

The results illustrate how the introduction of cycles (Family B) and modular attachments (Family C) systematically increases the number of matchings and alters growth behaviour relative to purely linear structures.

6.3 Comparative Analysis with Existing Indices

The sensitivity profile of Hosoya index is quite different than those exhibited by the classical distance-based topological indices, such as Wiener or Zagreb indices. Although distance-based indices are largely representative of the global separation of the vertex, Hosoya index is sensitive to the independence between edges and combinatorial flexibility. Consequently, the Hosoya index is able to discriminate between graphs having similar distance distributions but very different matching structures. It thus works very well in contexts where edge order, and not vertex distance, is the primary source of structure. Based on comparison, we assert that the Hosoya index is not a redundant measurement but complementary information with other indices.

6.4 Generalisations and Limitations

Several natural extensions of the present work can be identified. One promising direction is the study of weighted Hosoya indices, where edges or vertices are assigned, weights reflecting chemical or probabilistic properties. Another extension involves probabilistic matchings, in which matchings are sampled according to specified distributions, connecting the Hosoya index to statistical physics models. Applications to random graph models also present an interesting avenue for future research, particularly in understanding expected Hosoya index values and variance behaviour. A key limitation of the current methodology is the rapid growth of computational complexity for dense graphs or graphs with large boundary state spaces. While recurrence and transfer-matrix methods scale well for sparse and modular families, alternative approximation or asymptotic techniques may be required for highly connected graphs.

6.5 Applications and Implications in Chemical Graph Theory

In chemical graph theory, matchings correspond to sets of non-adjacent chemical bonds, and the Hosoya index has long been associated with molecular stability, branching, and resonance energy. The explicit formulas and recurrence relations derived in this study enable rapid and exact evaluation of the Hosoya index for molecular graphs modelled by the considered families. This is particularly relevant for polymer chains, benzenoid systems, and decorated molecular structures, where repeated subunits and pendant groups naturally arise. The results, therefore, support both theoretical analysis and practical computation in chemical informatics and molecular design.

7. Conclusions

In this paper, we have carried out a detailed and systematic study of the Hosoya index for specific classes of graphs whose constructions are based on matching structures. By combining structural decomposition techniques, recurrence-based analysis and state-oriented computation, we provided a comprehensive framework to study the counting of matchings in highly structured graph classes. The method focuses on the role of local combinatorial restrictions, in particular vertex and edge interactions and how they affect the global matching behaviour. For path-based structures (Family A), we showed that linear growth and local independence naturally imply low-order recurrence relations of Fibonacci kind, which in turn cause exponential growth determined by classical combinatorial sequences. On the other hand, the cyclic components in Family B change the recurrence structure and give Lucas-like behavior, showing that even minor topological changes can lead to major differences in some of these matching counts. For modularity core-attachment graphs (Family C), we established that boundary-state decompositions allow for systematic factorization or state-summing of the Hosoya index, and this reveals the effect of structural modularity in simplifying enumeration problems which are also generally complex and hard to treat. The comparative study across these families validates an important conclusion of this work: more than the maze topology and superficial graph geometry, matching constraints and structural dependencies dominate the growth behavior and qualitative aspects of the Hosoya index. Graphs sharing the same local matching rule display similar asymptotic growth behaviors despite their vastly different overall morphologies. These are supportive to the idea that the Hosoya index should be regarded as a structural index capturing more combinatorial than geometric information. The methodological framework proposed here combines classical recurrence-based approaches and a modular decomposition principle with computational test procedures. It forms a flexible tool that can be specialized to more general graph class, such as ladder graphs, cactus graphs and other inductively built families. Furthermore, the computational results verify the stability and scalability of recurrence-driven enumeration for small graph sizes, showing that it is a more practical approach than regular matching listing. A number of possible directions for future research occur quite naturally from this work. One interesting extension is the investigation of the weighted Hosoya indices, where edges or vertices have weights and represent chemical, probabilistic, or physical quantities. Another direction is probabilistic and random graph models where expected values and variance of the Hosoya index can uncover further structural information. Algebraically, more study on the interaction between Hosoya index, matching polynomials and spectral properties of graphs may shed some light on zeros distribution and asymptotic. From the chemical graph point of view, we have direct applicability in molecular modeling related directly to polymer chains, benzenoid-like structures and graphs with pendant substitutions. The methods of recurrence and decomposition developed here facilitate effective computation of all such matching-based descriptors for any family with iteratively-repeating substructures, facilitating both theoretical studies and practical applications in chemical informatics.

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