

TREES MAXIMIZING THE NUMBER OF ALMOST-PERFECT MATCHINGS

*Stijn Cambie, Bradley McCoy, Gunjan Sharma, Stephan Wagner and
Corrine Yap**

We characterize the extremal trees that maximize the number of almost-perfect matchings, which are matchings covering all but one or two vertices, and those that maximize the number of strong almost-perfect matchings, which are matchings missing only one or two leaves. We also determine the trees that minimize the number of maximal matchings. We apply these results to extremal problems on the weighted Hosoya index for several choices of vertex-degree-based weight function.

1. INTRODUCTION

A matching in a graph G is a set of edges such that no two edges share a vertex. Matching theory has a rich history with many applications. In particular, extremal problems and enumeration problems involving matchings have been studied extensively. A maximum matching can be the best solution to a variety of problems, such as scheduling and task assignment problems or matching donors with receivers [3, 12].

Computing the number of matchings in a graph, also called the Hosoya index, is #P-complete in general. In this paper, we focus on enumeration of matchings in trees. It is known that the number of matchings in the n -vertex path graph P_n is equal to F_n , the n th Fibonacci number (where $F_1 = 1, F_2 = 2$), and that this is the maximum over all n -vertex trees [6]. In fact, the star and the path respectively

*Corresponding author. Corrine Yap

2020 Mathematics Subject Classification. Primary 05C05, Secondary 05C09, 05C70.

Keywords and Phrases. Trees, Matching, Almost-perfect matching, Maximal matching, Weighted Hosoya index.

minimize and maximize not only the number of matchings but also the number of induced matchings [9], and the number of matchings of a fixed size [17, Thm. 4.7.3]. In the last case, we show that the path is, in fact, the unique maximizer. For a more comprehensive background on matching enumeration problems, see e.g. the survey of Wagner and Gutman [16], or the book by Wagner and Wang [17].

To prove that the path uniquely maximizes the number of matchings of a fixed size, we require results on almost-perfect matchings which are of independent interest. Perfect matchings are central to the study of matching theory—Hall’s matching theorem and Tutte’s theorem are perhaps the most notable examples [7, 15]. However, the notion of a matching that is “close to perfect” has been less prevalent. When the number of vertices in a graph is odd, an almost-perfect matching is a matching that avoids a single vertex. This is also called a near-perfect matching, and enumeration problems for other classes of graphs (such as factor-critical graphs and grid graphs) have been considered [2, 11, 13]. When the number of vertices is even, an almost-perfect matching avoids two vertices. We characterize the extremal trees in both cases and prove the following:

Theorem 1. *If n is odd, a tree T of order n has at most $\frac{n+1}{2}$ almost-perfect matchings. Equality holds if and only if T is a 1-subdivision of a tree of order $\frac{n+1}{2}$.*

Theorem 2. *If n is even, a tree T of order n has at most $\binom{\frac{n}{2}+1}{2} = \frac{n(n+2)}{8}$ almost-perfect matchings.*

- For $n > 4$, equality holds if and only if T is the path P_n .
- For $n = 4$, equality holds for both P_4 and S_4 .

We consider the same questions for strong almost-perfect matchings, which are matchings that cover all vertices except one or two leaves, and again find precise characterizations of the extremal graphs. When the order is odd, the number of strong almost-perfect matchings is maximized by the basic spider (a star with all but at most one edge subdivided once, as presented in Figure 1); this is the same construction that, for example, maximizes the number of maximal independent sets [18].

Theorem 3. *Let T be a tree of order $n \geq 28$. Then the number of strong almost-perfect matchings in T is at most $\frac{n-1}{2}$ if n is odd and $\lfloor \frac{(n-4)^2}{12} \rfloor$ if n is even. Equality holds if and only if T is a spider (when n is odd) or a balanced spider-trio (when n is even).*

In fact, we are able to give a complete picture of the bounds and extremal trees for all values of n , but postpone the precise statements until Section 4.

The trees that maximize the number of maximal matchings have been previously determined by Górska and Skupień [5]. Surprisingly, the characterization of the trees that minimize the number of maximal matchings has not appeared in the literature. We show that the extremal trees are precisely the most basic spiders again, or a special spider if n is odd.

Theorem 4. *A tree T of order n has at least $\lceil \frac{n}{2} \rceil$ maximal matchings. Equality holds if and only if T is a spider Sp_n , or an odd special spider SS_n .*

In Section 6, we consider applications to the weighted Hosoya index $Z_\phi(T)$, where each edge is assigned a weight by the function ϕ and the weight of a matching is the product of its edge weights. Motivated by recent results by Cruz, Gutman, and Rada [1], we consider certain choices of vertex-degree-based weight functions and prove that while the minimizer is the star in all cases that we consider, the maximizer can be the path, the double-broom, or a type of spider.

The outline of the paper is as follows: we start with mentioning some basics in Section 2. In Section 3, we prove Theorems 1 and 2. In Section 4, we prove Theorem 3. In Section 5, we prove Theorem 4. In Section 6, we prove results related to the weighted Hosoya index. We conclude by discussing some further questions to pursue in Section 7.

2. PRELIMINARIES

In this section, we introduce definitions and notation that will be used throughout the paper. Given a graph $G = (V, E)$, a *matching* M in G is a set of edges such that no two edges share a common vertex. A matching is *maximal* if it is not a subset of any other matching. A matching is a *maximum matching* if it has the largest possible cardinality. A *perfect* matching is a matching that includes all vertices.

The subgraph $G[V']$ of $G = (V, E)$ induced by a set $V' \subset V$ is the graph with vertex set V' and edge set $E \cap \binom{V'}{2}$. Two vertices u, v are adjacent (neighbors of each other) if $uv = (u, v) \in E$. This adjacency will also be denoted by $u \sim v$.

The *diameter* of a graph G , denoted $\text{diam}(G)$, is the maximum distance between any pair of vertices over all pairs in G . When we say “a diameter of G ,” we mean a path with length equal to $\text{diam}(G)$. A *1-subdivision of an edge* uv is obtained by adding a new vertex x_{uv} and replacing uv with the path $\{u, x_{uv}, v\}$. A *1-subdivision of a graph* is a graph all of whose edges are (1-)subdivided.

Definition 5. *In a tree of order n , a matching M is an almost-perfect matching (APM) if it covers all but one vertex when n is odd and all but two vertices when n is even. The vertices not covered by M are called the avoided vertices. M is a strong almost-perfect matching (SAPM) if the avoided vertices are leaves.*

Let $\mathcal{M}(G)$ be the set of all matchings of G , $\mathcal{M}_k(G)$ be the set of matchings in G of size k , and $m_k(G) = |\mathcal{M}_k(G)|$ with $m_0(G) = 1$. The *Hosoya index* of G is the number of matchings of G , which can be written as

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

The name of the index refers to Hosoya [8] who observed that if G is a molecular graph, the Hosoya index is correlated with its chemical properties.

Let (G, ω) denote a graph with weight function $\omega : E \rightarrow \mathbb{R}^+$. The weight of a matching M is then the product of the weights of the edges in M , and the *weighted Hosoya index* is

$$Z(G, \omega) = \sum_{M \in \mathcal{M}(G)} \left(\prod_{e \in M} \omega(e) \right).$$

Note that $\emptyset \in \mathcal{M}(G)$ for all G ; by convention we take the weight of the empty matching to be 1, so when viewed as a polynomial in $\{\omega(e)\}_{e \in E(G)}$, the weighted Hosoya index always has constant term 1. As an aside, observe that this coincides with the definition of the (multivariate) monomer-dimer partition function from statistical physics when $\omega(e)$ is a positive constant λ_e for each edge e .

Let $e = uv$ with $\deg(u) = i$ and $\deg(v) = j$. The weight function is *vertex-degree-based* if $\omega(e) = \phi(i, j)$ where ϕ is a function such that $\phi(i, j) = \phi(j, i)$. In this case, we denote $Z(G, \omega)$ by $Z_\phi(G)$.

We finish this section with some statements that we will use in our proofs throughout. We will refer to the fact $\sum_{v \in V(G)} \deg(v) = 2|E(G)|$ as the ‘‘handshaking lemma.’’ The following is also a well-known statement:

Lemma 6. *Every tree has at most one perfect matching.*

Proof. Suppose M and M' are two perfect matchings of T . In the graph $(V(T), M \cup M')$, every component must be either a single edge (contained in both M and M') or a cycle. As T is a tree, it contains no cycles and so we must have $M = M'$. \square

For two non-increasing sequences $x_1 \geq x_2 \geq \dots \geq x_k$ and $y_1 \geq y_2 \geq \dots \geq y_k$, we say $(x_i)_{i=1}^k$ *majorizes* $(y_i)_{i=1}^k$ if and only if $\sum_{i=1}^j x_i \geq \sum_{i=1}^j y_i$ for every $1 \leq j \leq k$ and equality holds for $j = k$. Analogously, for two non-decreasing sequences $x_1 \leq x_2 \leq \dots \leq x_k$ and $y_1 \leq y_2 \leq \dots \leq y_k$, we say $(x_i)_{i=1}^k$ *majorizes* $(y_i)_{i=1}^k$ if and only if $\sum_{i=1}^j x_i \leq \sum_{i=1}^j y_i$ for every $1 \leq j \leq k$ and equality holds for $j = k$.

Observe that if $(x_i)_{i=1}^k$ and $(y_i)_{i=1}^k$ are non-increasing, then the sequences $(x'_i)_{i=1}^k$ and $(y'_i)_{i=1}^k$ defined by $x'_i = x_{k-i+1}$ and $y'_i = y_{k-i+1}$ are non-decreasing, and $(x_i)_{i=1}^k$ majorizes $(y_i)_{i=1}^k$ if and only if $(x'_i)_{i=1}^k$ majorizes $(y'_i)_{i=1}^k$.

Our main use of this notion is the following inequality.

Lemma 7 (Karamata’s inequality, [10]). *If $(x_i)_{i=1}^k$ is a sequence of real numbers that majorizes $(y_i)_{i=1}^k$, and f is a real-valued convex function, then $\sum_{i=1}^k f(x_i) \geq \sum_{i=1}^k f(y_i)$. This inequality is strict if the sequences are not equal and f is a strictly convex function. If f is concave, the reverse inequality holds.*

3. MAXIMUM NUMBER OF MATCHINGS OF A FIXED SIZE

In this section, we characterize the trees T of order n maximizing the number of almost-perfect matchings and use this to characterize those maximizing the number of matchings of a fixed size k . When $n = 2k$, any tree with a perfect matching

is extremal since the perfect matching must be unique. While it is straightforward to check if a given tree has a perfect matching, there is not a clear characterization of the set of all trees with perfect matchings (there are exponentially many of them [14]).

When $n = 2k + 1$, we prove that there are many extremal trees maximizing the number of almost-perfect matchings. For convenience, we recall the theorem statement:

Theorem 1. *If n is odd, a tree T of order n has at most $\frac{n+1}{2}$ almost-perfect matchings. Equality holds if and only if T is a 1-subdivision of a tree of order $\frac{n+1}{2}$.*

Proof. Recall that every tree has a unique bipartition, so let $T = (X \cup Y, E)$. If T has an almost-perfect matching, then the bipartition classes must differ by 1 and the larger one, without loss of generality X , contains precisely $\frac{n+1}{2}$ vertices. This immediately implies the upper bound, since $T \setminus \{y\}$ for $y \in Y$ cannot have a perfect matching.

Next, we prove the characterization of the extremal trees. Let T' be an arbitrary tree of order $\frac{n+1}{2}$. Let T be a 1-subdivision of T' , with Y the set of added vertices. For every $v \in V(T')$, we can construct a perfect matching of $T \setminus \{v\}$: viewing T as a tree rooted at v , match each $u \in V(T') \setminus \{v\}$ with its neighbor (in Y) on the unique path from u to v . Hence any subdivision of a tree of order $\frac{n+1}{2}$ contains $\frac{n+1}{2}$ almost-perfect matchings.

We prove the other direction by induction on n . The cases $n \in \{1, 3\}$ are straightforward, since P_3 is the only tree of order 3 and is the 1-subdivision of P_2 . Thus, assume the statement is true for $n - 2$, where $n \geq 5$. Let $T = (X \cup Y, E)$ be a tree that attains equality and without loss of generality, let $|X| = \frac{n+1}{2}$. Then for every choice of $v \in X$, $T \setminus \{v\}$ has a perfect matching. Observe that every leaf of T must be in X . If there is a leaf in Y , then its unique neighbor in X cannot be avoided by an almost-perfect matching, since any such matching would also avoid the leaf itself. This implies that no two leaves can have the same neighbor. Indeed, if $x_1, x_2 \in X$ are leaves, then for any $v \in X$ such that $v \neq x_1, x_2$, the almost-perfect matching that avoids v would have to cover both leaves x_1 and x_2 , a contradiction.

Now let $x \in X$ be a leaf such that its unique neighbor y has degree 2 (such a leaf must exist, e.g. one of the ends of a diameter). Then $T' := T \setminus \{x, y\}$ is a tree. Furthermore, for any $v \in X \setminus \{x\}$, we know that $T \setminus \{v\}$ has a perfect matching, which must contain the edge xy . Thus, T' contains $\frac{n-1}{2}$ almost-perfect matchings so we may apply the inductive hypothesis to conclude that T' is a 1-subdivision of a tree, and hence T is as well. \square

Next, we will show that when $n = 2k + 2$, the path is extremal in all non-trivial cases. We start with a lemma that will be applied in the proof of this and some further theorems.

Lemma 8. *If n is even and T is a tree of order n with at least one pair of leaves sharing a common neighbor, then T has at most $n - 1$ almost-perfect matchings.*

Proof. Recall that for n even, an almost-perfect matching M covers all but two vertices, and we call these vertices the avoided pair of M . Let T be a tree of order n , and let u and u' be the two leaves with a common neighbor (siblings). No matching can cover both leaves, so for every almost-perfect matching M of T , at least one of u and u' is contained in the avoided pair of M .

By Theorem 1, $T \setminus \{u\}$ and $T \setminus \{u'\}$ have both at most $\frac{n}{2}$ almost-perfect matchings. Equality is only possible if $T \setminus \{u\}$ and $T \setminus \{u'\}$ are 1-subdivisions of a tree. Since the perfect matching of $T \setminus \{u, u'\}$ has been counted twice, T has at most $n - 1$ almost-perfect matchings. Because $T \setminus \{u\}$ and $T \setminus \{u'\}$ are isomorphic, we also know that equality is attained if and only if T is a 1-subdivision of a tree of order $\frac{n}{2}$ where one copy of a leaf is added (i.e. a copy u' of a leaf u with the same neighbor). \square

We use this to prove the case for n even:

Theorem 2. *If n is even, a tree T of order n has at most $\binom{\frac{n}{2}+1}{2} = \frac{n(n+2)}{8}$ almost-perfect matchings.*

- For $n > 4$, equality holds if and only if T is the path P_n .
- For $n = 4$, equality holds for both P_4 and S_4 .

Proof. One can check by hand that for $n = 4$ both P_4 and S_4 have three almost-perfect matchings, for $n = 6$ the path P_6 has six almost-perfect matchings, and in both cases these are the only examples attaining the maximum.

Now let $n \geq 8$ and suppose the claim holds for all even numbers less than or equal to $n - 2$.

Since $n < \frac{n(n+2)}{8}$, by Lemma 8 we may assume there are no two leaves with a common neighbor. Taking a diameter of the tree, we note that there is an edge uv with u a leaf and v its neighbor of degree 2. Then either uv is contained in the almost-perfect matching, or the avoided pair contains u . We count the number of matchings in each case and take the sum to get the total number of almost-perfect matchings in T .

For the first term, the number of almost-perfect matchings containing uv is equal to the number of almost-perfect matchings in $T \setminus \{u, v\}$ which by the inductive hypothesis is at most $\frac{n(n-2)}{8}$. For the second term, the number of avoided pairs containing u is at most the number of almost-perfect matchings in $T \setminus \{u\}$, which is bounded by $\frac{(n-1)+1}{2}$ by Theorem 1. Since $\frac{n(n-2)}{8} + \frac{(n-1)+1}{2} = \frac{n(n+2)}{8}$, the first statement of the theorem holds by induction.

To characterize equality, we see by the inductive hypothesis that equality holds for the first term if and only if $T \setminus \{u, v\} = P_{n-2}$. By Theorem 1, equality holds for the second term if and only if $T \setminus \{u\}$ is a 1-subdivision of a tree of order $\frac{n}{2}$. Since v must have degree 2, these imply that equality holds overall if and only if $T = P_n$. \square

Another way of stating Theorem 2 is that P_n maximizes $m_k(T)$ when $n = 2k + 2$ and $k \geq 2$. We can extend this to larger values of n . Note that $m_1(T) = n - 1$ for every tree T and so it has been omitted in the statement.

Theorem 9. *If $k \geq 2$ and T is a tree of order n with $n \geq 2k + 2$, then $m_k(T) \leq m_k(P_n) = \binom{n-k}{k}$. Equality holds if and only if $T = P_n$.*

Proof. We will prove that the statement is true for forests of order n using induction on k .

When $k = 2$, for a tree T we have $m_2(T) = \binom{n-1}{2} - \sum_v \binom{\deg(v)}{2}$. Observe that the degree sequence of the path P_n is majorized by the degree sequence of any other n -vertex tree. Indeed, the degree sequence of P_n is $(2, 2, \dots, 2, 1, 1)$. If $T \neq P_n$ has degree sequence $(d_1 \geq d_2 \geq \dots \geq d_n)$ and $\sum_{i=1}^j d_i < 2j$ for some $j \leq n - 2$, then we must have $d_i = 1$ for all $i \geq j$. Then $\sum_{i=1}^n d_i < 2j + (n - j) \leq 2n - 2$, a contradiction since $\sum_{i=1}^n d_i = 2(n - 1)$ by the handshaking lemma. Thus, we may apply Lemma 7 (with strict inequality since the degree sequences of T and P_n must be different) to conclude that for any $T \neq P_n$, we have $m_2(T) < m_2(P_n) = \binom{n-2}{2}$.

If F is a forest with at least two components, then $|E(F)| \leq n - 2$ and as such, $m_2(F) \leq \binom{n-2}{2}$. Equality is not possible when $n > 4$.

Now assume the statement holds for $m_{k-1}(T)$ for any T on $n \geq 2k$ vertices. When $n = 2k + 2$, a matching of size k is an almost-perfect matching and so P_n is extremal among trees by Theorem 2. For a forest F with multiple components, there are three cases.

Case 1: All components of F have even size. Let the components of F be T_1, T_2, \dots, T_r where $|T_i| = 2k_i$ for $1 \leq i \leq r$. An almost-perfect matching of F consists of an almost-perfect matching of T_i for some i and a perfect matching of T_j for every $j \neq i$, of which there is at most one by Lemma 6. Then

$$m_k(F) \leq \sum_{i=1}^r m_{k_i-1}(T_i) \leq \sum_i m_{k_i-1}(P_{2k_i}).$$

We claim this is strictly less than $m_k(P_n)$. By Theorem 2, it suffices to observe that

$$\sum_{i=1}^r \binom{k_i + 1}{2} < \binom{\sum k_i + 1}{2}.$$

This is true by induction on r since $\binom{a+b+1}{2} > \binom{a+1}{2} + \binom{b+1}{2}$ for every $a, b \geq 1$ (a straightforward computation).

Case 2: At least four components are odd. Then $m_k(F) = 0$ since at least one vertex from each of the four components must be avoided.

Case 3: Exactly two components are odd, with order a and b . In the last case, we apply Theorem 1 and the inequality between the arithmetic and geometric mean (AM-GM) to conclude $m_k(F) \leq \frac{a+1}{2} \cdot \frac{b+1}{2} \leq \left(\frac{k+2}{2}\right)^2 < \binom{k+2}{2} = m_k(P_n)$. Thus, the statement is true for forests when $n = 2k + 2$.

So for $n \geq 2k + 3$, we may assume that the claim holds for $n - 1$.

Let F be a forest and u a leaf of F , with unique neighbor v (a forest without edges is clearly not extremal). We observe that $m_k(F) = m_k(F \setminus \{u\}) + m_{k-1}(F \setminus \{u, v\})$, since either u is covered by the matching or it is not. By the inductive hypothesis, we have that $m_k(F \setminus \{u\})$ is maximized when $F \setminus u = P_{n-1}$ and $m_{k-1}(F \setminus \{u, v\})$ is maximized when $F \setminus \{u, v\} = P_{n-2}$. This shows that $m_k(F)$ is maximized if and only if $F = P_n$, completing the induction. \square

4. MAXIMUM NUMBER OF STRONG ALMOST-PERFECT MATCHINGS

Recall that a strong almost-perfect matching (SAPM) is a matching which avoids one leaf when n is odd and two leaves when n is even. In this section, we characterize the trees that maximize the number of SAPMs with three theorems which, combined, give a more complete version of Theorem 3.

We first define the relevant families of trees. Often a spider can refer to any subdivision of a star, i.e. any tree which has at most one vertex of degree at least 3. We will refer to a spider Sp_n as the unique spider of order n whose “legs” all have length 2, except possibly one leg of length 1 when n is even.

Definition 10. *An odd spider is a 1-subdivision of a star. It has odd order. An even spider is an odd spider with an additional pendant edge added to the unique vertex of degree ≥ 3 , or added to the center of a P_5 . It has even order. We use the notation Sp_n for a (odd or even depending on parity of n) spider of order n . See Figure 1. A spider Sp_i for $i \leq 5$ corresponds with a path P_i .*

A leg then refers to any of the 1-subdivided edges or to the additional pendant edge.

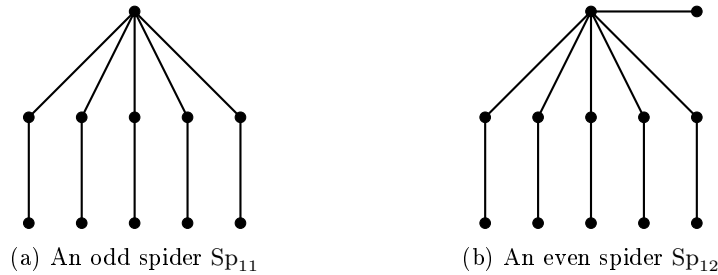


Figure 1: Two spiders

Definition 11. *A double broom $DB_{a,b}$ is a tree of diameter 3 whose non-leaves have degree $a + 1$ and $b + 1$ respectively. A balanced double broom on n vertices is a tree of diameter 3 whose non-leaves have degree $\lfloor \frac{n}{2} \rfloor$ on one side and $\lceil \frac{n}{2} \rceil$ on the other side. See Figure 2a.*

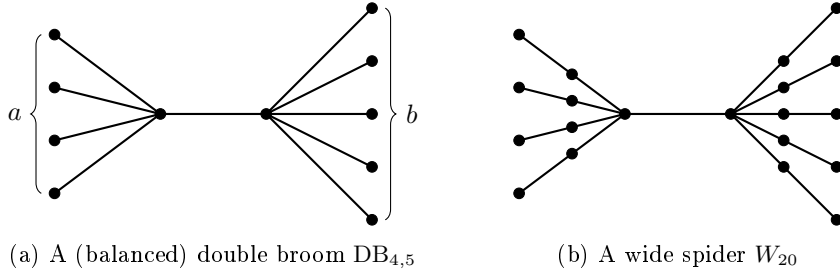


Figure 2: A double broom and wide spider

Theorem 12. *Let n be odd. If $n \geq 5$, a tree T of order n has at most $\frac{n-1}{2}$ strong almost-perfect matchings.*

For $n \geq 7$, equality holds if and only if T is an odd spider.

For $n = 5$, equality holds for both $DB_{1,2}$ and P_5 .

Proof. If T is a tree that contains two leaves with a common neighbor, then T has at most two SAPMs, since every matching must avoid at least one of these two leaves. Otherwise, T has at least as many internal vertices as leaves and thus at most $\frac{n-1}{2}$ leaves. It follows that T has at most $\frac{n-1}{2}$ SAPMs. The n -vertex spider achieves this upper bound.

For $n = 5$, we have $\frac{n-1}{2} = 2$, and one can check by hand that the extremal graphs are the path P_5 (which is a spider) and the double broom $DB_{1,2}$. For $n \geq 7$, let T be a tree of order n with $\frac{n-1}{2}$ SAPMs. Then T must have $\frac{n-1}{2}$ leaves $\{u_i : 1 \leq i \leq \frac{n-1}{2}\}$. For each i , let v_i be the unique neighbor of u_i . This gives us $n - 1$ vertices, so T contains one additional vertex x . For each i , $T \setminus \{u_i\}$ has a perfect matching, which must contain $u_j v_j$ for all $j \neq i$. Thus, $x \sim v_i$ for all i , and so T is indeed a spider. \square

When n is even, an almost-perfect matching M of T contains all but two vertices, so counting the number of almost-perfect matchings of T is equivalent to counting the number of avoided pairs $P \subset V(T)$ for which $T \setminus P$ has a perfect matching. This is the strategy we employ to prove the next theorem, in which we have the additional assumption that T contains a perfect matching.

Definition 13. *A wide spider is constructed by subdividing every pendant edge of a double broom. For $n = 2k$, the balanced wide spider W_n on n vertices is the tree one obtains from subdividing every pendant edge of a balanced double broom on $k + 1$ vertices. See Figure 2b.*

Theorem 14. *Let n be even. If T is a tree of order n that contains a perfect matching, then the number of strong almost-perfect matchings in T is at most*

$$\max \left\{ 1, \frac{n-2}{2}, \left\lfloor \frac{(n-2)^2}{16} \right\rfloor \right\} = \begin{cases} 1 & n = 2, \\ \frac{n-2}{2} & 2 < n \leq 10, \\ \left\lfloor \frac{(n-2)^2}{16} \right\rfloor & n \geq 10. \end{cases}$$

Equality holds if and only if either

- $n \leq 10$, and T is obtained by attaching a leaf to each vertex of a tree of order $\frac{n}{2}$, or
- $n \geq 10$, and T is the balanced wide spider.

Proof. If $n = 2$, then there is precisely one SAPM, namely the empty matching, so assume that $n > 2$. Let T be an arbitrary tree of order n with a perfect matching. Let $\{u_1, \dots, u_k\}$ be the leaves of T . Observe that no two leaves have the same neighbor; else, the perfect matching would match both with their common neighbor. It follows that $k \leq \frac{n}{2}$. Let v_i be the unique neighbor of u_i , $1 \leq i \leq k$.

Recall that a bipartite graph can have a perfect matching only if the parts of the bipartition are the same size. Consider the (unique) bipartition $V(T) = X \cup Y$. An SAPM of T that avoids u_i and u_j is a perfect matching of $T \setminus \{u_i, u_j\}$. This can occur only if u_i and u_j belong to different parts of the bipartition $X \cup Y$. Thus, there are at most $\left\lfloor \frac{k^2}{4} \right\rfloor$ SAPMs of T .

If $k = \frac{n}{2}$, then $T[\{v_1, \dots, v_k\}]$ must be a tree of order $\frac{n}{2}$, and every SAPM in T can only avoid u_i and u_j such that $v_i \sim v_j$. This gives $\frac{n}{2} - 1 = \frac{n-2}{2}$ SAPMs in T , one for each edge of $T[\{v_1, \dots, v_k\}]$.

Otherwise, $k \leq \frac{n}{2} - 1 = \frac{n-2}{2}$, which means that there are at most $\left\lfloor \frac{(n-2)^2}{16} \right\rfloor$ SAPMs. This is achieved by the wide spider W_n . Indeed, for every pair of leaves on opposite sides, there is an APM that avoids those leaves, so the number of SAPMs in W_n is $\left\lfloor \frac{(n-2)^2}{16} \right\rfloor$.

Thus, we have shown that the maximum is

$$\max \left\{ 1, \frac{n-2}{2}, \left\lfloor \frac{(n-2)^2}{16} \right\rfloor \right\},$$

and it remains to discuss the cases of equality. Note first that $\frac{n-2}{2} \geq \left\lfloor \frac{(n-2)^2}{16} \right\rfloor$ if and only if $n \leq 10$ (with equality for $n = 10$), so the case that there are $k = \frac{n}{2}$ leaves yields the maximum for $2 < n \leq 10$, while the case that there are $k = \frac{n}{2} - 1$ leaves and $\left\lfloor \frac{k^2}{4} \right\rfloor$ SAPMs yields the maximum for $n \geq 10$.

It only remains to show that the wide spider W_n is unique in the second case. Suppose T has $k = \frac{n-2}{2}$ leaves and $\left\lfloor \frac{(n-2)^2}{16} \right\rfloor$ almost-perfect matchings. Let x and

y be the two vertices that are neither leaves nor neighbors of leaves. Their degree is at least 2. The perfect matching of T must contain the edge $u_i v_i$ for all i , so $x \sim y$. Suppose without loss of generality that $x \in X, y \in Y$. Then there is some $v_i \in X, v_j \in Y$ such that $x \sim v_j$ and $y \sim v_i$.

Let $v_\ell \in X$ for $\ell \neq i$. Suppose for the sake of contradiction that $v_\ell \not\sim y$. For each m such that $v_m \in Y$, in order to have a perfect matching of $T \setminus \{u_\ell, u_m\}$, we must have $v_\ell \sim v_m$. This implies $v_m \not\sim x$ for all $m \neq j$; else, $\{x, v_j, v_\ell, v_m\}$ would form a cycle. Then there cannot be an almost-perfect matching that avoids u_i and u_m for $m \neq j$, since there is no disjoint set of edges to cover v_m, v_ℓ , and u_ℓ , which is a contradiction. This tells us that $v_\ell \sim y$ for all ℓ such that $v_\ell \in X$, and a similar argument shows that $v_m \sim x$ for all m such that $v_m \in Y$, and so T is isomorphic to the balanced wide spider. \square

When we remove the requirement that T contains a perfect matching, we can still characterize the extremal examples as follows:

Definition 15. An even special spider SS_n on n vertices for n even is an odd spider Sp_{n-1} with a sibling added for one of the leaves. See Figure 3a.

A spider trio $ST_{a,b,c}$ is a tree constructed from three odd spiders $Sp_{2a+1}, Sp_{2b+1}, Sp_{2c+1}$ whose center vertices are attached to a single new vertex. See Figure 3b.

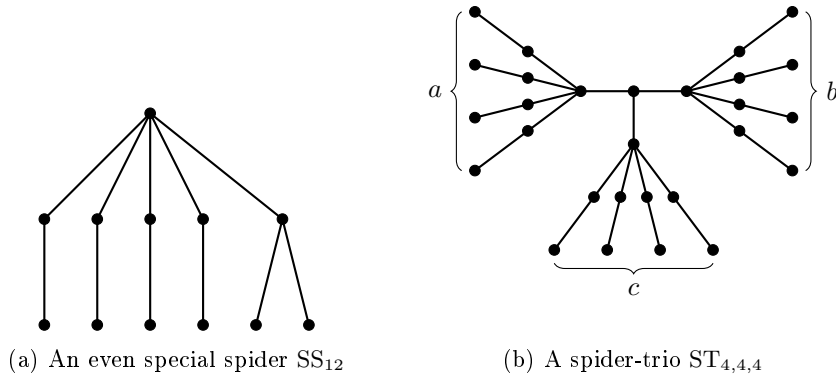


Figure 3: Other variants of spiders

Theorem 16. Let $f(n)$ be the maximum number of SAPMs in a tree T of order n . Then, for n even,

$$f(n) = \begin{cases} \lfloor \frac{3n}{4} \rfloor & \text{if } 2 \leq n \leq 6, \\ n - 3 & \text{if } 8 \leq n \leq 14, \\ \lfloor \frac{n^2}{16} \rfloor - 1 & \text{if } 16 \leq n \leq 28, \\ \lfloor \frac{(n-4)^2}{12} \rfloor & \text{if } n \geq 30. \end{cases}$$

Equality holds if and only if T is one of the following trees:

$$\begin{cases} P_2, S_4, \text{ or } DB_{2,2} & \text{for } 2 \leq n \leq 6, \\ SS_n & \text{if } 8 \leq n \leq 12, \\ SS_{14} \text{ or } ST_{3,2,0} & \text{if } n = 14, \\ ST_{\lceil \frac{n-4}{4} \rceil, \lfloor \frac{n-4}{4} \rfloor, 0} & \text{if } 16 \leq n \leq 26, \\ ST_{6,6,0} \text{ or } ST_{4,4,4} & \text{if } n = 28, \\ ST_{\lfloor \frac{n}{6} \rfloor, \lfloor \frac{n-2}{6} \rfloor, \lfloor \frac{n-4}{6} \rfloor} & \text{if } n \geq 30. \end{cases}$$

Proof. For $n \leq 16$, the values of $f(n)$ have been checked with a computer, so we may assume $n \geq 18$. Let T be a tree on n vertices. If two leaves of T share a common neighbor, then by Lemma 8, T has at most $n - 1$ SAPMs. Since $f(n) > n$ (as evidenced by the trees given in the claim), T cannot be extremal in this case.

Thus, we may also assume that every leaf has a unique neighbor and so the number of leaves is at most $\frac{n}{2}$. If T has exactly $\frac{n}{2}$ leaves, then T must also contain a perfect matching. By Theorem 14, T has at most $\lfloor \frac{(n-2)^2}{16} \rfloor$ SAPMs, which is smaller than both $\lfloor \frac{n^2}{16} \rfloor - 1$ and $\lfloor \frac{(n-4)^2}{12} \rfloor$ when $n \geq 18$.

Now suppose the number of leaves in T is at most $\frac{n}{2} - 1$. Let $V(T) = X \cup Y$ be the bipartition of T , and without loss of generality, suppose $|X| \geq |Y|$. Recall that T containing an almost-perfect matching implies that either $|X| = |Y|$ or $|X| = |Y| + 2$. If $|X| = |Y|$, then every avoided pair of leaves must have one element in X and one element in Y . There are at most $\lfloor \frac{(n-2)^2}{16} \rfloor$ such pairs, which again is less than the stated upper bounds.

So now we assume that $|X| = |Y| + 2 = \frac{n}{2} + 1$.

Case 1: Y contains no leaves. Then the degree of every vertex in Y is at least 2. As $|Y| = \frac{n-2}{2}$, and $\sum_{v \in Y} \deg(v) = n - 1$, this implies that all but one vertex in Y has degree 2. Let z be the unique vertex in Y which has degree 3.

In that case $T \setminus \{z\}$ has three components—call them A, B, C . Each component is itself a tree whose vertices in Y have degree 2. Thus each of them has one more vertex in X than in Y . In particular, each component has an odd number of vertices in total.

Observe that if a component, say C , of $T \setminus \{z\}$ does not contain a member of the avoided pair, then, since $|C|$ is odd, the SAPM must match z with its neighbor in C . Thus, an avoided pair of leaves cannot be contained in a single component.

Let a, b, c be the number of leaves in A, B , and C respectively, with $a \geq b \geq c$. Then the number of SAPMs is bounded above by $ab + bc + ac$. If B and C are singletons, this gives an upper bound of $1 + 2a < n$. If only C is a singleton, then we have $ab + a + b = (a + 1)(b + 1) - 1 \leq \lfloor \frac{n^2}{16} \rfloor - 1$. Furthermore, we can see that equality is attained only for the tree $ST_{a,b,0}$ when $a = b = \frac{n}{4}$. Indeed, each SAPM of T is a union of SAPMs of A and B , and the edge from z to C . By Theorem 12, A and B have the maximum number of SAPMs if and only if they are both spiders.

Else, each neighbor of z is a non-leaf vertex in X , and as such $a+b+c \leq \frac{n-4}{2}$. By the AM-GM inequality, we know that $ab+bc+ac \leq \frac{(a+b+c)^2}{3}$ and since the number of SAPMs is an integer, we conclude that $\lfloor \frac{(n-4)^2}{12} \rfloor$ is an upper bound. By an argument similar to the previous case, the extremal tree is precisely the balanced spider-trio $ST_{a,b,c}$ where $a \geq b \geq c \geq a-1$. This has exactly $\lfloor \frac{(n-4)^2}{12} \rfloor$ SAPMs. It is now sufficient to note that $\lfloor \frac{n^2}{16} \rfloor - 1 \leq \lfloor \frac{(n-4)^2}{12} \rfloor$ if and only if $n \geq 28$.

Case 2: There is a leaf $y \in Y$. Let x be the unique neighbor of Y . Since $|X| = |Y| + 2$, every avoided pair must be contained in X and so every almost-perfect matching must contain xy .

If $\deg(x) = 2$, the number of SAPMs of T equals the number of SAPMs of $T \setminus \{x, y\}$, which is at most $f(n-2)$. It is straightforward to verify algebraically that $\lfloor \frac{n^2}{16} \rfloor - 1$ (for $16 \leq n \leq 28$) and $\lfloor \frac{(n-4)^2}{12} \rfloor$ (for $n \geq 28$) are increasing functions, so the result follows by induction.

If $\deg(x) > 2$ and $T \setminus \{x, y\}$ is a forest, the result also follows similarly by induction since $T \setminus \{x, y\}$ is a subgraph of a tree. If the components of $T \setminus \{x, y\}$ are all even, with orders n_1, n_2, \dots, n_k , then there is some $i \in \{1, \dots, k\}$ such that the component of order n_i has two more vertices in X than in Y . This implies that T has at most $f(n_i) < f(n)$ SAPMs. If two components are odd, we have at most $\lfloor \frac{(n-2)^2}{16} \rfloor$ pairs of leaves, one in each odd component. Therefore, there are at most $\lfloor \frac{(n-2)^2}{16} \rfloor \leq \lfloor \frac{(n-4)^2}{12} \rfloor$ SAPMs. □

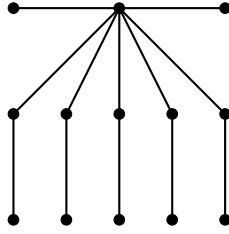
5. MINIMUM NUMBER OF MAXIMAL MATCHINGS

In this section, we characterize trees with the minimum number of maximal matchings. This complements the result of Górska and Skupień [5] on the maximum number of maximal matchings.

Definition 17. *An odd special spider SS_n on n vertices for n odd is an even spider Sp_{n-1} with a pendant edge added to the center vertex (for $n \geq 7$, this is the unique vertex of degree ≥ 3). See Figure 4.*

Theorem 4. *A tree T of order n has at least $\lceil \frac{n}{2} \rceil$ maximal matchings. Equality holds if and only if T is a spider Sp_n , or an odd special spider SS_n .*

Proof. We proceed by induction on n . A small computer verification confirms the claim for $n \leq 7$ (the paths P_n are also spiders Sp_n when $n \leq 5$). Now let $n \geq 8$. We consider two cases. First, suppose there are two leaves u_1, u_2 with a common neighbor v . Let $T' = T \setminus \{u_1, u_2\}$. Observe that every maximal matching M of T' can be extended to a maximal matching of T . If M covers v , then M is also a maximal matching of T . If M does not cover v , then we can extend M with u_1v or with u_2v . Thus, T has at least as many maximal matchings as T' .

Figure 4: An odd special spider SS_n where $n = 13$

In the second case, no two leaves share a common neighbor. Then there must exist a leaf u whose unique neighbor v has degree 2 (for example, suppose T is rooted at an arbitrary vertex ρ and take u to be a leaf at maximum depth). Let $T' = T \setminus \{u, v\}$ and let x be the other neighbor of v . As before, every maximal matching M of T' can be extended to a maximal matching of T and so T has at least as many maximal matchings as T' . Indeed, if M covers x , the unique extension is given by $M \cup \{uv\}$. If M does not cover x , we can extend using either uv or vx .

Moreover, in both cases, we can always find a maximal matching of T that uses a particular edge not contained in T' (either u_1v or u_2v in the first case, and either uv or vx in the second case). This shows that T has strictly more maximal matchings than T' , and we conclude by induction.

For equality to be attained by T , equality needs to be attained by T' and thus T' is a spider or an odd special spider. Note that T' has at least two legs of length 2 and thus T has at least one leg of length 2, say with leaf vertex y and neighbor z . By applying the inductive hypothesis to $T \setminus \{y, z\}$, we know that $T \setminus \{y, z\}$ has to be either Sp_{n-2} , or SS_{n-2} if n is odd. We can then conclude that T itself is Sp_n or SS_n , and these indeed attain equality. \square

Initially, this question about determining the minimum number of maximal matchings was motivated by the following observation about maximal matchings, which we will utilize in applications to the weighted Hosoya index. We say the *degree sum* of a maximal matching M to mean $\sum_{v \in V(M)} \deg(v)$.

Lemma 18. *If $n \geq 2$, then the degree sum of a maximal matching M in a tree T of order n is at least n . Equality occurs only if T is a star, or T has diameter 3 and M is the central edge.*

Note that the statement is trivially false for a 1-vertex tree, so $n \geq 2$ is required.

Proof. Let M be a maximal matching. If $v \in V$ is not covered by M , then there must exist some $u \in N(v)$ that is covered by M ; else, $M \cup \{uv\}$ is a larger matching, contradicting the maximality of M . This implies that $\bigcup\{N(u) : u \text{ is covered by } M\} = V$, from which the statement follows.

Equality can occur only if every vertex has precisely one neighbor covered by the matching. By the argument above, for every v not covered by M , we must have all of $N(v)$ covered by M . This implies that all non-leaf vertices of T are covered by M . If the diameter of T is at least 4, then there exist internal vertices of a diameter path which have more than one neighbor covered by M , and so equality does not occur. If T has diameter 3, there are only two types of maximal matchings and we conclude easily. \square

As a corollary of Theorem 4 and Lemma 18, we have the following result on the weighted Hosoya index. This is a special case of a more general theorem that we prove in the next section. Recall that S_n denotes the n -vertex star.

Corollary 19. *Let $\phi(i, j) = c^{i+j}$ where $c \geq 2$. Then for every n -vertex tree T , we have $Z_\phi(S_n) \leq Z_\phi(T)$.*

Proof. First note that S_n has $n - 1$ nonempty matchings, each with weight c^n , so $Z_\phi(S_n) = (n - 1)c^n + 1$. For a tree T that is not a star, by Theorem 4, T has at least $\lceil \frac{n}{2} \rceil$ maximal matchings. By Lemma 18, each maximal matching has degree sum strictly greater than n , with possibly one exception which has degree sum exactly equal to n . Thus we have $Z_\phi(T) > (\lceil \frac{n}{2} \rceil - 1)c^{n+1} + c^n + 1 \geq (n - 1)c^n + 1 = Z_\phi(S_n)$. The first inequality is strict since there are pendant edges which are not maximal matchings and contribute in the sum as well. The second inequality holds by our assumption $c \geq 2$. \square

6. EXTREMAL VALUES OF THE WEIGHTED HOSOYA INDEX

Recall that the weighted Hosoya index is defined to be

$$Z(T, \omega) = \sum_{M \in \mathcal{M}(T)} \prod_{e \in M} \omega(e)$$

where the weight of the empty matching is 1. In this section, we characterize the extremal examples for some natural choices of weights that are vertex-degree-based, meaning $\omega(e) = \phi(i, j)$ where i and j are the degrees of the endpoints of e . We then write $Z(T, \omega)$ as $Z_\phi(T)$.

We consider the following weight functions for $c > 0$:

$$\begin{aligned} \phi_1(i, j) &= c^{i+j}, \\ \phi_2(i, j) &= c^{ij}, \\ \phi_3(i, j) &= (i + j)^c, \\ \phi_4(i, j) &= (ij)^c. \end{aligned}$$

Note that these examples are all symmetric in i and j . It was shown in [1] that for $c < 0$, the star minimizes the weighted Hosoya index for ϕ_3 and ϕ_4 (also referred

to as the general Randić index and general sum-connectivity index, respectively). This can also be derived from the following proof that the star minimizes the weighted Hosoya index for $c > 0$.

Theorem 20. *Let $c > 0$. Then for every n -vertex tree T , we have $Z_{\phi_\ell}(T) \geq Z_{\phi_\ell}(S_n)$ for all $\ell \in \{1, 2, 3, 4\}$. Equality holds in each case if and only if $T = S_n$.*

Proof. Let $Z_\phi(T, v, k)$ be the weighted Hosoya index of T where the weight of v is increased by k . That is, if $uv = e \in E(T)$ for some u , then $\omega(e) = \phi(\deg(u), \deg(v) + k)$. We will use induction to prove a stronger statement:

Claim 21. *Let T be a tree on n vertices, and let $v \in V(T)$ be a non-leaf vertex that has at least one leaf neighbor. For any nonnegative integer k and $\ell \in \{1, 2, 3, 4\}$, $Z_{\phi_\ell}(T, v, k) \geq Z_{\phi_\ell}(S_n, x, k)$ where x is the center vertex of the star.*

Observe that taking $k = 0$ gives the theorem statement.

We proceed by induction on n . We can check the first non-trivial base case ($n = 4$) directly to see that the claim holds true for all $k \geq 0$ and all $c > 0$.

Now suppose that for every $n' < n$, the claim holds for all $k \geq 0$.

Let T be an n -vertex tree different from S_n , and let k be a nonnegative integer. Let $v \in T$ be a non-leaf vertex. Let u_1, \dots, u_s be the $s \geq 1$ leaf neighbors of v and let x_1, \dots, x_t be the non-leaf neighbors. Let T_i be the component of x_i in $T \setminus \{v, u_1, \dots, u_s\}$. Then

$$(1) \quad Z_\phi(T, v, k) = Z_\phi(T \setminus \{u_1, \dots, u_s\}, v, s + k) + s\phi(1, \deg(v) + k) \prod_{i=1}^t Z_\phi(T_i, x_i, 1).$$

Given a star graph S_n , let z_n denote the center vertex.

First consider $\phi_1(i, j) = c^{i+j}$. We can calculate that $Z_{\phi_1}(S_n, z_n, k) = (n - 1)c^{n+k} + 1$. By (1) and the inductive hypothesis,

$$\begin{aligned} Z_{\phi_1}(T, v, k) &\geq Z_{\phi_1}(S_{n-s}, z_{n-s}, s + k) + s\phi_1(1, s + t + k) \prod_{i=1}^t Z_{\phi_1}(S_{|T_i|}, z_{|T_i|}, 1) \\ &\geq (n - s - 1)c^{(n-s)+(s+k)} + 1 + sc^{(s+t)+k+1} \prod_{i=1}^t ((|T_i| - 1)c^{|T_i|+1} + 1). \end{aligned}$$

Observe that $\sum_{i=1}^t |T_i| = n - s - 1$, so we have

$$\begin{aligned} Z_{\phi_1}(T, v, k) &\geq (n - s - 1)c^{n+k} + 1 + sc^{s+t+k+1} \left(c^{(n-s-1)+t} \prod_{i=1}^t (|T_i| - 1) + 1 \right) \\ &= (n - s - 1)c^{n+k} + 1 + sc^{n+2t+k} \prod_{i=1}^t (|T_i| - 1) + sc^{s+t+k+1}. \end{aligned}$$

We want the last expression to be at least $(n-1)c^{n+k} + 1$. Recall that $s \geq 1$ by assumption. Dividing both sides of the desired inequality by sc^{n+k} and rearranging, it suffices to show

$$c^{2t} \prod_{i=1}^t (|T_i| - 1) + c^{s+t+1-n} \geq 1.$$

If T is not isomorphic to S_n , then $t \geq 1$ and $|T_i| \geq 2$ for all i , so when $c \geq 1$, the first term is at least 1 and the inequality holds. The second term is also positive, so the inequality must be strict in this case.

When $c < 1$, we use that $n = (s+1) + \sum_{i=1}^t |T_i| \geq s+1+2t$, so the second term is at least 1, and as before, the inequality holds and is strict for $T \neq S_n$.

(As a remark, note that a more direct argument works for ϕ_1 in the case $c < 1$. Since T is a tree, $\deg(u) + \deg(v) \leq n$ for every edge uv in T . Thus, $Z_{\phi_1}(T) \geq (n-1)c^n + 1$ where equality holds if and only if T is the star. However, this argument does not apply to the case of, for example, $\phi_2(i, j) = c^{ij}$.)

The calculations are almost identical for ϕ_2, ϕ_3 , and ϕ_4 , so we omit many of the details here. Each computation begins by applying (1) and the inductive hypothesis.

For ϕ_2 , we have $Z_{\phi_2}(S_n, z_n, k) = (n-1)c^{n+k-1} + 1$ whereas for general T , we have

$$Z_{\phi_2}(T, v, k) \geq (n-s-1)c^{n+k-1} + 1 + sc^{n+t+k-1} \prod (|T_i| - 1) + sc^{s+t+k}$$

and similarly to the case of ϕ_1 , we can show that this is at least $(n-1)c^{n+k-1} + 1$ with equality if and only if $T = S_n$.

For ϕ_3 , we have $Z_{\phi_3}(S_n, z_n, k) = (n-1)(n+k)^c + 1$ and on the other hand

$$Z_{\phi_3}(T, v, k) \geq (n-s-1)(n+k)^c + 1 + s(s+t+k+1)^c \prod (|T_i| + 1)^c.$$

Since $n+k < n+k+t = (s+t+k) + \sum |T_i| + 1$ and each of the terms $(s+t+k)$ and $\sum |T_i|$ is at least 2, we know that $n+k \leq (s+t+k+1) \prod (|T_i| + 1)$ and so

$$Z_{\phi_3}(T, v, k) \geq (n-s-1)(n+k)^c + 1 + s(n+k)^c = (n-1)(n+k)^c + 1$$

as desired.

Lastly, for ϕ_4 , we have $Z_{\phi_4}(S_n, z_n, k) = (n-1)(n+k-1)^c + 1$ and

$$Z_{\phi_4}(T, v, k) \geq (n-s-1)(n+k-1)^c + 1 + s(s+t+k)^c \prod (|T_i|)^c.$$

Similar to the previous case, the result follows from $n+k-1 \leq (s+t+k) \prod |T_i|$. \square

From this and previous work on the Hosoya index, one might be tempted to conjecture that the path and the star are always extremal, even if not uniquely so. It turns out this is not the case. Recall the definitions of the double-broom $DB_{a,b}$ (11) and the wide spider W_n (13).

Theorem 22. *For c sufficiently large in terms of n , the tree that (uniquely) maximizes $Z_{\phi_\ell}(T)$ among all trees of order n is*

- $\ell = 1$: W_n if $n \geq 12$ is even and Sp_n if $n \geq 7$ is odd,
- $\ell = 2$: $\text{DB}_{\lfloor \frac{n}{2} \rfloor - 1, \lceil \frac{n}{2} \rceil - 1}$ if $n \geq 6$,
- $\ell \in \{3, 4\}$: P_n .

Proof for ϕ_1 . Recall that $\phi_1(i, j) = c^{i+j}$. Suppose first that n is even. For a perfect matching M , we must have

$$\sum_{e=uv \in M} (\deg(u) + \deg(v)) = 2(n - 1).$$

Thus, for $c \geq 1$, the leading term of $Z_{\phi_1}(T)$ is at most c^{2n-2} (since every tree has at most one perfect matching). The second leading term corresponds to the weight of strong almost-perfect matchings in T , which must each have weight c^{2n-4} . Because we are taking c sufficiently large, it is enough to recall from Theorem 14 that the balanced wide spider uniquely maximizes the number of SAPMs for $n \geq 12$.

If n is odd, the leading term of $Z_{\phi_1}(T)$ is given by SAPMs which each have weight c^{2n-3} . From Theorem 12, we know that the odd spider has the maximum number of SAPMs when $n \geq 7$. \square

Proof for ϕ_2 . To prove the result for $\phi_2(i, j) = c^{ij}$ we use the following claim.

Claim 23. *Let T be a tree of order $n \geq 6$ and M a matching of T . Then $\sum_{uv \in M} \deg(u) \cdot \deg(v) \leq \lfloor \frac{n^2}{4} \rfloor$, with equality if and only if T is the balanced double-broom $\text{DB}_{\lfloor \frac{n}{2} \rfloor - 1, \lceil \frac{n}{2} \rceil - 1}$ with diameter 3 and M consists of the central edge.*

Proof of Claim. Let $M = \{e_1, \dots, e_k\}$ and for every i , let d_i be the sum of the degrees of the endpoints of e_i . Assume the edges are ordered such that $d_1 \leq d_2 \leq \dots \leq d_k$. Since $n > 2$, we know $d_i \geq 3$ for every i . There are $n - 2k$ vertices not covered by M , so by the handshaking lemma, we know that $\sum_{i=1}^k d_i \leq 2(n - 1) - (n - 2k) = n + 2k - 2$. If $k = 1$, then M consists of a single edge uv and by the AM-GM inequality,

$$\deg(u) \deg(v) \leq \left\lfloor \frac{d_1^2}{4} \right\rfloor \leq \left\lfloor \frac{n^2}{4} \right\rfloor.$$

When $k \geq 2$, it suffices to prove that

$$\sum_i \left\lfloor \frac{d_i^2}{4} \right\rfloor \leq \left\lfloor \frac{n^2}{4} \right\rfloor.$$

In this case, we apply Lemma 7. Consider the sequences $A = (3, 3, \dots, 3, \sum_{i=1}^k d_i - 3(k - 1))$ with the first $k - 1$ terms equal to 3, and $B = (d_1, \dots, d_k)$. Both sequences

sum to $\sum_{i=1}^k d_i$ and since $d_i \geq 3$ for all i , we have that for any $\ell < k$, the sum of the first ℓ terms of A is at most the sum of the first ℓ terms of B . This means that A majorizes B , so we may apply Karamata's inequality with the convex function $f(x) = x^2$ to get that $\sum_{i=1}^k d_i^2 \leq (k-1)3^2 + ((n+2k-2) - 3(k-1))^2 = n^2 - (k-1)(2n-k-8) < n^2 - 1$, where we use that $n \geq \max\{6, 2k\}$ and conclude.

Since the last inequality is strict, equality cannot be achieved by any matching of size at least two. In the case $k = 1$, the extremal tree must contain an edge whose endpoints each have degree $\frac{n}{2}$; the balanced double-broom is the unique example. \diamond

Now let T be a tree of order n such that $T \neq \text{DB}_{\lfloor \frac{n}{2} \rfloor - 1, \lceil \frac{n}{2} \rceil - 1}$. We know that $|\mathcal{M}(T)| \leq F_n$, the n th Fibonacci number. Thus,

$$Z_{\phi_2}(T) \leq F_n c^{\lfloor \frac{n^2}{4} \rfloor - 1} < c^{\lfloor \frac{n^2}{4} \rfloor} < Z_{\phi_2}\left(\text{DB}_{\lfloor \frac{n}{2} \rfloor - 1, \lceil \frac{n}{2} \rceil - 1}\right)$$

where the second inequality requires our assumption that c is sufficiently large in terms of n . \square

Proof for ϕ_3 . For $\phi_3(i, j) = (i + j)^c$, the leading term of Z_{ϕ_3} does not correspond with a unique graph. We first prove a general claim about maximizing the product of a set of integers, which follows from Karamata's inequality.

Claim 24. *Assume integers a_1, a_2, \dots, a_k sum to $qk + r$, where $0 \leq r < k$. Then $\prod_{i=1}^k a_i \leq (q+1)^r q^{k-r}$ and equality occurs only if r of the a_i s equal $q+1$ and $k-r$ of them equal q .*

Proof. Let the a_i s be ordered such that $a_1 \geq a_2 \geq \dots \geq a_k$. Then $\sum_{i=1}^{\ell} a_i \geq \ell(q+1)$ for every $\ell \leq r$. If not, $a_i \leq q$ for every $i \geq \ell$ and thus $\sum_{i=1}^k a_i \leq \ell(q+1) - 1 + (k-\ell)q < kq + \ell \leq kq + r$, a contradiction. Similarly, the sum of the $\ell \leq k-r$ smallest values among the a_i s is bounded by ℓq . This implies that the sequence (a_1, a_2, \dots, a_k) majorizes the sequence

$$\left(\underbrace{q+1, q+1, \dots, q+1}_r, \underbrace{q, q, \dots, q}_{k-r} \right).$$

By Lemma 7 applied to the concave function $\log(x)$, we conclude that $\sum_i \log(a_i) \leq r \log(q+1) + (k-r) \log(q)$. \diamond

Claim 25. *Let T be a tree of order $n \geq 4$ and M a matching in T . Then*

$$\prod_{uv \in M} (\deg(u) + \deg(v)) \leq \begin{cases} 3^2 \cdot 4^{(n-4)/2} & \text{if } n \text{ is even,} \\ 3 \cdot 4^{(n-3)/2} & \text{if } n \text{ is odd.} \end{cases}$$

Equality is possible only if M is a perfect matching (for n even) or strong almost-perfect matching (for n odd). Moreover, for all other matchings the upper bound can be reduced by a factor of 2.

Proof of Claim. Let $V = \{v_1, \dots, v_n\}$ be an arbitrary permutation of the vertices and $d_i = \deg(v_{2i-1}) + \deg(v_{2i})$ (observe that $v_{2i-1}v_{2i}$ is not necessarily an edge of T). If $n = 2k$ is even, then $\sum_{i=1}^k d_i = 2n - 2 = 4k - 2$ by the handshaking lemma and by Claim 24, $\prod_{i=1}^k d_i \leq 3^2 \cdot 4^{k-2}$. Equality happens only when all d_i are 3 or 4. If M is not a perfect matching and covers vertices $\{v_1, \dots, v_{2m}\}$ (without loss of generality), then $2m < 2k$ so we may divide both sides by $d_k \geq 2$ to get the final part of the claim.

If $n = 2k+1$ is odd, then $\sum_{i=1}^k d_i \leq 2(n-1) - 1 = 4k - 1$ and $\prod_{i=1}^k d_i \leq 3 \cdot 4^{k-1}$ by Claim 24. Similar arguments hold for equality and when M is not an SAPM as in the even case. \diamond

We say uv is an (a, b) -edge if $\deg(u) = a, \deg(v) = b$. To determine which tree achieves equality in the previous claim, a trivial but crucial observation is that $\deg(u) + \deg(v) = 4$ if and only if uv is a $(2, 2)$ - or $(3, 1)$ -edge. The path P_n is a tree that attains equality in Claim 25, but not the unique one.

First, consider the case where $n = 2k + 1$ is odd. The leading terms for $Z_{\phi_3}(P_n)$ are $2 \cdot (3 \cdot 4^{k-1})^c + (k - 1) \cdot (3^2 \cdot 4^{k-2})^c$.

Let $T \neq P_n$ be a tree of order n . The (strong) almost-perfect matching(s) for which equality is attained in Claim 25 consist of $(3, 1)$ - and $(2, 2)$ -edges with exactly one $(2, 1)$ -edge. Observe that the extremal tree must then consist of a central path (the diameter) with pendant leaves connected to the internal vertices. There are at most two choices for an SAPM that attains equality in Claim 25. If there is only one $(2, 1)$ -edge in T (an example is presented in Figure 5 on the left), then there are two leaves with the same neighbor of degree 3 and hence only 2 APM's in total (since an APM must contain exactly one of the two neighboring leaves). That implies whenever c is sufficiently large that

$$Z_{\phi_3}(T) < 2 \cdot (3 \cdot 4^{k-1})^c + F_n \cdot (3 \cdot 4^{k-1}/2)^c < Z_{\phi_3}(P_n).$$

If there are two $(2, 1)$ -edges in T , let u and v be the two leaves at the end of the diameter. Observe that we cannot have perfect matchings of both $T \setminus \{u\}$ and $T \setminus \{v\}$; this is because T has a $(3, 1)$ -edge (since $T \neq P_n$) which must be contained in both matchings. Deleting the endpoints of the $(3, 1)$ -edge splits the tree into two components, both of which have odd order in one of $T \setminus \{u\}$ or $T \setminus \{v\}$. So, in this case there is at most one matching for which equality in Claim 25 holds. Thus the leading term in $Z_{\phi_3}(T)$ is smaller than $2 \cdot (3 \cdot 4^{k-1})^c$ and the result follows again.



Figure 5: Trees for which $Z_{\phi_3}(T)$ and $Z_{\phi_3}(P_n)$ have the same leading term

Next, we consider the case where n is even. A tree T that attains equality in Claim 25 has maximum degree at most 3, every vertex of degree 3 has a neighboring

leaf, and T has a perfect matching (see the right hand side of Figure 5 for an example). As before, T consists of a diameter with pendant leaves. The second largest contribution to $Z_{\phi_3}(T)$ would be due to a strong almost-perfect matching M , for which $\prod_{uv \in M} (\deg(u) + \deg(v)) \leq 2^{n-2}$ by Claim 25, and equality occurs only if the avoided pair are the endpoints of the diameter, and the degree 3 vertices in M are paired with leaves.

Let the diameter have vertices v_1, v_2, \dots, v_k where $\{v_1, v_k\}$ is the avoided pair, and let i be minimum such that $\deg(v_i) = 3$. In order for M to cover the vertices v_2, \dots, v_{i-1} , we must have i even. But T has a perfect matching, and in order for the perfect matching to cover v_1, v_2, \dots, v_{i-1} , we must have i odd - a contradiction unless T contains no vertices of degree 3, i.e. $T = P_n$. \square

Proof for ϕ_4 . Finally, to prove the result for $\phi_4(i, j) = (ij)^c$ we use the following claim.

Claim 26. *Let T be a tree on $n \geq 2$ vertices. Then the product of the degrees of all vertices is at most 2^{n-2} , with equality if and only if T is a path P_n .*

Proof. A tree has at least 2 leaves, so by the handshaking lemma the other $n - 2$ vertices have degree 2 on average. The claim follows from the AM-GM inequality and the fact that the path is the only tree with exactly two leaves. \diamond

As such, the leading term of $Z_{\phi_4}(P_n)$ is $(2^{n-2})^c$, while for any other tree T of order n , we have $Z_{\phi_4}(T) \leq F_n (3 \cdot 2^{n-4})^c$, which is smaller than $(2^{n-2})^c$ once e.g. $c > 2n$. \square

7. FURTHER DIRECTIONS

We conclude with some further open problems.

7.1 Maximum number of strong k -almost-perfect matchings for $k \geq 3$

We can generalize the notion of an almost-perfect matching to a *k -almost-perfect matching* (k -APM), a matching which covers all but k vertices. Similarly, a *strong k -almost-perfect matching* (k -SAPM) covers all but k leaves. Observe that $k \in \{1, 2\}$ recovers our original notion of APM and SAPM. For $k \geq 3$, we can consider the question of which trees have the maximum number of k -SAPMs.

Recall a spider is the unique tree of order n whose legs all have length 2, except possibly one leg of length 1 when n is even and a spider-trio is a tree constructed from three spiders whose center vertices are attached to a single new vertex. In Theorem 16, for n sufficiently large, we showed that the spider-trio maximizes the number of SAPMs. For n sufficiently large, one could hope that a generalized $(k + 1)$ -spider, presented in Figure 6 for $k = 7$, is extremal. This might be true for

small k , but is false for $k \geq 13$. When $k = 13$ a tree consisting of spiders connected to a path has more k -SAPMs than the $(k + 1)$ -spider. Asymptotically, however, the generalized $(k + 1)$ -spider has the optimal order.

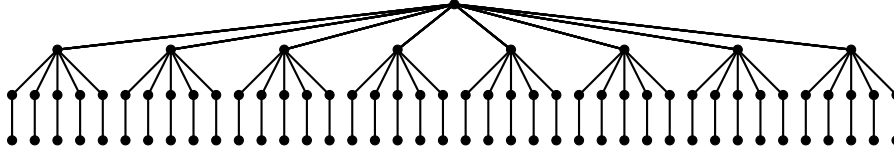


Figure 6: A generalized 8-spider

Proposition 27. *The number of strong k -almost-perfect matchings in a tree of order n is $\Theta_k(n^k)$.*

Proof. The number of k -SAPMs is bounded by $\binom{n}{k} = O_k(n^k)$. For the lower bound, let T be the union of $k + 1$ odd spiders all of order $2a + 1$, whose centers are connected with an additional vertex v as in Figure 6. Then $n = (k + 1)(2a + 1) + 1$ and the number of k -SAPMs in T is $(k + 1)a^k \sim \frac{n^k}{2^{k(k+1)^{k-1}}} = \Omega_k(n^k)$. \square

We can also determine some structural properties that the extremal tree(s) must have.

Proposition 28. *If T contains two leaves that share a common neighbor, then the number of strong k -almost-perfect matchings is at most $2\binom{n}{k-1} = O(n^{k-1})$.*

Proof. If two leaves, ℓ_1 and ℓ_2 , have the same neighbor, then no matching can contain both of them. Thus, in any k -APM at least one of the two is in the avoided set of k leaves. For both ℓ_1 and ℓ_2 , the number of k -APMs is bounded by the number of ways to choose the remaining $k - 1$ leaves to avoid. \square

As a consequence, for n sufficiently large, we can partition the vertices into three sets: the set of leaves L , the set of (unique) neighbors of the leaves $N := N(L)$ and the set of vertices X that are at distance at least two from any leaf. Observe that $|L| = |N|$ and $|X| + 2|L| = n$. For a subset of vertices S , let $T[S]$ denote the subtree induced by S .

Proposition 29. *The number of strong k -almost-perfect matchings that contain an edge in $T[N]$ is $O_k(n^{k-1})$.*

Proof. A k -SAPM M is uniquely determined by the avoided set of k leaves. If there is an edge in $T[N] \cap M$, then the endpoints have neighbors in L which must also be in the avoided set, together with $k - 2$ other leaves. There are fewer than $n - 1$ edges in $T[N]$ and $O(n^{k-2})$ choices for the other $k - 2$ leaves, which results in a total of $O(n^{k-1})$ k -SAPMs that contain an edge in $T[N]$. \square

Thus, there are few k -SAPMs that contain an edge between two vertices in N . We suspect the extremal trees are spiders connected to a relatively small X , but the structure of X seems difficult to characterize. Surprisingly, when $T[X]$ is a path, the optimal number of leaves in each spider is not monotone as the following example illustrates.

Example 30. *When T is the union of 8 spiders whose centers are connected with a path, such that T is symmetric, the number of strong 4-APM's is maximized when the ratios of their sizes (counted from outer to inner spiders) is approximately $\frac{27}{16} : 1 : \frac{9}{16} : \frac{3}{4}$.*

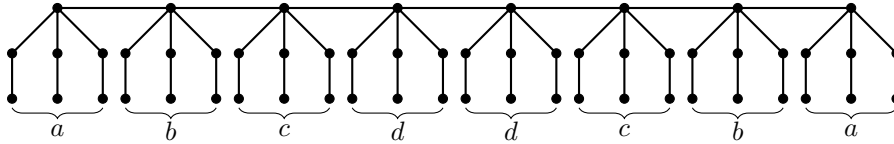


Figure 7: A construction where $T[X] = P_8$

To see this, let the number of leaves of the 8 spiders be a, b, c, d, d, c, b, a respectively, as presented in Figure 7. Then $2(a + b + c + d) = \frac{n-8}{2}$. A strong 4-APM can only be obtained when taking four leaves from different spiders in such a way that the centers of the other four form a matching in the path. The total number of choices for these leaves is equal to $(b^2 + (2c + 2d)b + d^2)a^2 + 2c((c + 2d)b + d^2)a + c^2d^2$. Using a small computer verification¹, we conclude that this homogenous multivariate polynomial is maximized when $(a : b : c : d) = (\frac{27}{16} : 1 : \frac{9}{16} : \frac{3}{4})$.

The preceding discussion may provide some intuition to tackle the following question:

Question 31. *For $k \geq 3$, characterize the trees which maximize the number of strong k -almost-perfect matchings.*

We can generalize the notion of k -SAPM even further to that of a *connected matching*, which is a matching M in a tree T such that $T[V(M)]$ is a connected graph. The notion of connected matching (among some other variants) was defined in [4]. Observe that every k -SAPM is a connected matching. Conversely, when n is odd, a connected matching with $\frac{n-1}{2}$ edges is an SAPM. One could ask similar questions about characterizing the extremal trees for connected matchings. It may be interesting to consider these type of questions for connected matchings in general graphs as well, or classes such as d -regular graphs which are well-studied in matching theory.

¹https://github.com/StijnCambie/MRC_trees_projects, document OptimalDistributionBehaviour.

7.2 Weighted Hosoya index

Regarding applications to the weighted Hosoya index, it would be interesting to determine the extremal trees for various other choices of degree-based weight function. In particular, can we characterize when the path and the star are the maximizer and minimizer, respectively?

For example, consider the function

$$\phi(i, j) = \varphi^{16 \lfloor \frac{ij}{16} \rfloor}$$

where φ is the golden ratio. While this choice of weight function may seem rather artificial, it is interesting to note that neither P_n nor S_n are extremal; one can check that $Z_\phi(P_n) = F_n \sim \varphi^n$ and $Z_\phi(S_n) \sim (n - 1)\varphi^{n-1}$. Here F_n is the n^{th} Fibonacci number. In fact, a weight of at least approximately $\varphi^{8n/3}$ can be achieved by the construction in Figure 8a below.

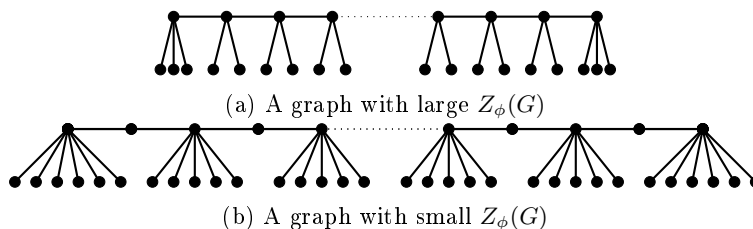


Figure 8: Two trees indicating that P_n and S_n are not extremal

On the other hand, a weight of at most $8^{n/7} < \varphi^{3n/4}$ is given by the construction in Figure 8b.

One might try to generalize the results of Section 6 to answer the following:

Question 32. *Can we fully characterize the class of functions ϕ for which $Z_\phi(T)$ is minimized by the star, or maximized by the path?*

Acknowledgments The authors would like to express their gratitude to the American Mathematical Society for organizing the Mathematics Research Community workshops where this work began, in the workshop “Trees in Many Contexts,” and to Wanda Payne for contributing to the initial discussions. This event was supported by the National Science Foundation under Grant Number DMS 1916439.

The first author has been supported by the Institute for Basic Science (IBS-R029-C4) and a postdoctoral fellowship by the Research Foundation Flanders (FWO) with grant number 1225224N. The fourth author was supported by the Knut and Alice Wallenberg Foundation (KAW 2017.0112) and the Swedish research council (VR), grant 2022-04030.

REFERENCES

1. R. CRUZ, I. GUTMAN, AND J. RADA: *Hosoya index of VDB-weighted graphs*. Discrete Appl. Math., **317** (2022), 18–25.
2. R. DOROSLOVAČKI, J. ĐOKIĆ, B. PANTIĆ, AND O. BODROŽA-PANTIĆ: *A conjecture concerning near-perfect matchings on $C_m \times P_n$ cylinders of odd order*. Appl. Anal. Discrete Math., **13**(2) (2019), 361–377.
3. D. GALE AND L. SHAPLEY: *College admissions and the stability of marriage*. Amer. Math. Monthly, **69**(1) (1962), 9–14.
4. W. GODDARD, S. M. HEDETNIEMI, S. T. HEDETNIEMI, AND R. LASKAR: *Generalized subgraph-restricted matchings in graphs*. Discrete Math., **293**(1-3) (2005), 129–138.
5. J. GÓRSKA AND Z. SKUPIEŃ: *Trees with maximum number of maximal matchings*. Discrete Math., **307**(11-12) (2007), 1367–1377.
6. I. GUTMAN: *Graphs with greatest number of matchings*. Publ. Inst. Math. (Beograd) (N.S.), **27**(41) (1980), 67–76.
7. P. HALL: *On representatives of subsets*. J. London Math. Soc., **10** (1935), 26–30.
8. H. HOSOYA: *Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons*. Bull. Chem. Soc. Jpn., **44**(9) (1971), 2332–2339.
9. D. Y. KANG, J. KIM, Y. KIM, AND H.-F. LAW: *On the number of r -matchings in a tree*. Electron. J. Combin., **24**(1) (2017), Paper No. 1.24, 16 pages.
10. J. KARAMATA: *Sur une inégalité relative aux fonctions convexes*. Publ. Math. Univ. Belgrade, **1** (1932), 145–148.
11. Y. LIU AND J. HAO: *The enumeration of near-perfect matchings of factor-critical graphs*. Discrete Math., **243**(1-3) (2002), 259–266.
12. L. LOVÁSZ AND M. D. PLUMMER: *Matching theory*. Volume 121 of North-Holland Mathematics Studies. North-Holland Publishing Co., Amsterdam, 1986.
13. S. N. PEREPECHKO: *Counting near-perfect matchings on $C_m \times C_n$ tori of odd order in the Maple system*. Program. Comput. Softw., **45**(2) (2019), 65–72.
14. R. SIMION: *Trees with 1-factors and oriented trees*. Discrete Math., **88**(1) (1991), 93–104.
15. W. T. TUTTE: *The factorization of linear graphs*. J. London Math. Soc., **22** (1947), 107–111.
16. S. WAGNER AND I. GUTMAN: *Maxima and minima of the Hosoya index and the Merrifield-Simmons index: a survey of results and techniques*. Acta Appl. Math., **112**(3) (2010), 323–346.
17. S. WAGNER AND H. WANG: *Introduction to chemical graph theory*. Discrete Mathematics and its Applications (Boca Raton). CRC Press, Boca Raton, FL, 2019.
18. H. S. WILF: *The number of maximal independent sets in a tree*. SIAM J. Algebraic Discrete Methods, **7**(1) (1986), 125–130.

Stijn Cambie

Department of Computer Science,
KU Leuven Campus Kulak-Kortrijk,
Kortrijk, Belgium
E-mail: *stijn.cambie@hotmail.com*

(Received 24. 08. 2023.)

(Revised 09. 03. 2025.)

Bradley McCoy

Department of Computer Science,
James Madison University,
Harrisonburg, VA, USA
E-mail: *mccoy2ba@jmu.edu*

Gunjan Sharma

Applied Mathematics,
Illinois Institute of Technology,
Chicago, IL, USA
E-mail: *gsharma7@hawk.iit.edu*

Stephan Wagner

Institute of Discrete Mathematics,
TU Graz,
Graz, Austria
and
Department of Mathematics,
Uppsala University,
Uppsala, Sweden
E-mail: *stephan.wagner@tugraz.at*

Corrine Yap

School of Mathematics,
Georgia Institute of Technology,
Atlanta, GA, USA
E-mail: *math@corrineyap.com*