Properties of graph polynomials and related parameters

by

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Abstract

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In this thesis, we investigate various problems related to graph polynomials. We first define two-variable polynomials for rooted trees and specific posets, which are motivated by the Tutte polynomial. We observe that these polynomials also satisfy a deletion-contraction property, and they are connected to antichains and transversals.

The second problem concerns the average size of independent vertex sets of a graph, following the work of Jamison on subtrees. The average size of independent sets is the logarithmic derivative of the independence polynomial evaluated at one. We characterize extremal graphs among all n-vertex graphs and all n-vertex trees for this invariant.

In a similar way, the average size of independent edge sets, also called matchings, is studied. We discover that graphs which minimize this invariant, maximize the average size of independent sets and vice versa. These results are expected, in view of the correlation between independent sets and matchings. Furthermore, we find a bound on the matching energy of a graph in terms of the average size of matchings.

Finally, we focus on a special class of trees, namely trees with given degree sequence. Many authors have already worked on different invariants for trees with prescribed degree sequence using quite diverse techniques. One surprising fact is that extremal trees for different parameters coincide.

Our goal is to generalise and unify these results within one proof. We rediscover known results for invariants such as the Wiener index, the number of subtrees, the matching polynomial and the number of independent sets, and also find new ones, as for rooted spanning forests, related to coefficients of the Laplacian polynomial, and the solvability of a graph.

Uittreksel

Eienskappe van grafiekpolinome en verwante parameters

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In hierdie tesis ondersoek ons verskeie probleme in verband met grafiekpolinome. Ons definieer eers ′n polinoom in twee veranderlikes vir gewortelde bome en spesifieke parsieel geordende versamelings, wat gemotveer is deur die Tutte-polinoom. Ons sien dat hierdie polinome ook ′n verwydering-kontraksie-eienskap bevredig, en hulle hou verband met antikettings en transversale.

Die tweede probleem gaan oor die gemiddelde grootte van onafhanklike versamelings van punte in ′n grafiek, waar ons die werk van Jamison oor deelbome volg. Die gemiddelde grootte van onafhanklike versamelings is die logaritmiese afgeleide van die onafhanklikheidspolinoom wat by een geëvalueer word. Ons karakteriseer die grafieke en bome met n punte wat die ekstreemwaardes bereik.

Op ′n soortgelyke manier word die gemiddelde grootte van onafhanklike versamelings van lyne, wat ook as matchings bekendstaan, bestudeer. Ons vind dat grafieke wat hierdie invariant se minimale waarde bereik, gelyktydig die gemiddelde grootte van onafhanklike puntversamelings maksimeer, en andersom. Hierdie resultate kan verwag word in die lig van die verband tussen onafhanklike versamelings en matchings. Verder vind ons ′n grens vir die energie van ′n grafiek in terme van die gemiddelde grootte van matchings.

Uiteindelik fokus ons op ’n spesiale klas bome, naamlik bome met gegewe graadry. Baie navorsers het reeds aan verskillende invariante gewerk vir bome met voorgeskrewe graadry deur gebruik te maak van redelik diverse tegnieke. Een verrassende feit is dat ekstremale bome vir verskillende parameters ooreenstem. Ons doelwit is om hierdie resultate in een bewys te veralgemeen en te verenig. Ons herontdek bekende resultate vir invariante soos die Wiener-indeks, die aantal deelbome, die matching-polinoom en die aantal onafhanklike versamelings, en vind ook nuwes, soos vir gewortelde spanbosse, wat verband hou met koëffisiënte van die Laplace-polinoom, en die oplosbaarheid van ’n grafiek.

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My profound gratitude goes to my beloved husband, for being constantly by my side in all challenges I had to overcome during these three years. Special thanks to my son, for being my main motivation.

“O give thanks unto the Lord; for he is good: for his mercy endureth for ever." Psalm 136,1

Dedications

To the memory of my dad Andriamandimby Razanajatovo,

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Chapter 1

Introduction

Graph polynomials are polynomials connected to graphs. They are tools to analyze properties of graphs and to encode information on the graph structures. Several graph polynomials have already been thoroughly studied in the literature, some of the most popular are the characteristic polynomial, the matching polynomial, the Laplacian polynomial and the Tutte polynomial. In this thesis, we treat various problems related to graph polynomials. This dissertation is made up of six chapters, where Chapter 2 provides basic definitions and terminologies used throughout the work.

The first problem concerns the Tutte polynomial. Namely, in Chapter 3, we investigate a Tutte-like polynomial for rooted trees and specific posets. We show that our polynomials can be described by means of a deletion-contraction recursion as for the Tutte polynomial [57]. Furthermore, we find a connection to the structure of the graphs. The Tutte-polynomial is associated to spanning subgraphs, while our polynomials are related to (maximal) antichains and transversals. These parameters are mainly defined for rooted trees, we may refer to [8, 41]. We end this chapter by enumerating the posets we work on.

In Chapter 4, we consider the average size of independent sets in a graph. This invariant is the logarithmic derivative of the independence polynomial evaluated at one. One of our motivation is the work of Jamison [37], on the average order of subtrees, but we substitute subtrees by independent sets. We show that although the average size of independent sets is not monotone, under adding or removing an edge, like the number of independent sets, the extremal graphs remain the same for general graphs and the class of trees. More explicitly, we find that this invariant is minimized (maximized) by the complete graph K_n (empty graph E_n) among all n-vertex graphs, and it is minimized (maximized) by the path P_n (star S_n) among all n-vertex trees. Furthermore, we studied also the weighted average size of independent sets, that is the logarithmic derivative of the independence polynomial at α up to a factor α, where α is a positive real number. We still obtain the same extremal graphs for any positive α, except for the path P_n, where we obtain a similar result as for the actual average size of independent sets only when $\alpha \in (0, 1]$.

In a similar line as Chapter 4, Chapter 5 concerns the average size of independent edge sets, also called matchings, in a graph. It is not surprising that the extremal graphs for the average size of independents sets and for the average size of matchings coincide for general graphs and trees. We will see that the average size of matchings is minimized (maximized) by E_n (K_n) among all n-vertex graphs, and it is minimized (maximized) by P_n (S_n) among all n-vertex trees. Besides, we get identical results for the weighted average size of matchings, where the extremality of E_n, K_n and S_n remain true for any positive α. However, P_n only maximizes the weighted average size of matchings for $\alpha \in (0, 1]$. In this chapter, we are also interested in a relation between the average size of matchings and the matching energy. Gutman and Wagner introduced the matching energy in [30], they observed that it is strongly connected to the matching polynomial of a graph. Thus, we expect a link between the average size of matchings and the matching energy. We indeed find a bound on the matching energy in terms of the average size of matchings.

The last problem, identified in Chapter 6, involves a particular class of trees. We are interested in characterizing extremal trees with a given degree sequence. This restriction on the degree is often used in mathematical chemistry, where the skeleton of an atom may be considered as a graph. Several invariants have already been investigated for this specific restriction, we may cite the Wiener index [53, 66], the number of subtrees [3, 74], independent sets [1] and so forth. A fascinating observation, is that the extremal trees for these distinct parameters coincide. We intend to unify those results within one proof. We observe that the extremal trees for a specific invariant often satisfy an exchange-extremal property associated to this invariant. Our method consists of generalising the lemma on exchange-extremality from [1, 34]. Namely, we associate a function to a particular invariant.

If this function is increasing (decreasing), combined with the fact that the exchange-extremal property is fulfilled, then our extremal tree is the greedy tree (the alternatingly greedy tree). We rediscovered known results as for the Wiener index, the terminal Wiener index, the number of subtrees, the matching polynomial, the number of independent sets, and the energy, but also obtain new ones as for the number of spanning rooted forests, which are related to the coefficients of the Laplacian polynomial, the incidence energy, and the solvability of a graph. Furthermore, we also generalize the results to trees with bounded degree sequences through majorization.

Chapter 2

Terminologies and basic notions

In this chapter, we provide terminologies and basic notions on graph theory that we make use of in the next chapters. All results presented can be found in standard books on graph theory, see for instance [4, 10, 19].

2.1 Basic notions

Definition 2.1.1. A *graph* is a pair of sets $(V(G), E(G))$, where the elements of $V(G)$ are called vertices of G, and the elements of $E(G)$, which are two-element subsets of $V(G)$, are called edges of G. $|V(G)|$ is the order of G and $|E(G)|$ its size. For simplicity an edge $\{u, v\}$ will be denoted by uv. The vertices u and v are said to be *adjacent* if uv is an edge and the edge uv is *incident* to u and v.

We sometimes use the longer notion of "simple undirected graph" for a graph as defined above to emphasize the fact that a graph does not contain loops, i.e., edges that join a vertex to itself, nor multiple edges between two vertices, and its edges do not have a direction. All graphs considered throughout the whole thesis will be simple and undirected graphs, unless mentioned otherwise.

Definition 2.1.2. Two graphs G and G' are *isomorphic* ($G \cong G'$) if we can find a bijection $\ell : V(G) \to V(G')$ such that $uv \in E(G) \iff \ell(u)\ell(v) \in E(G')$.

Definition 2.1.3. A graph G' is a *subgraph* of G if $V(G') \subseteq V(G)$ and $E(G') \subseteq E(G)$.

If in particular $V(G) = V(G')$, then G' is called a *spanning* subgraph of G.

Remark 2.1.4. Let $\{v_1, v_2, \ldots, v_k\}$ be a subset of the vertices of a graph G.

We denote by $G - \{v_1, v_2, \ldots, v_k\}$ the subgraph of G which results from removing the vertices $v_1, v_2, \ldots, v_k$ as well as the edges incidents to them.

In a similar way, we denote by $G - \{v_1w_1, \ldots, v_kw_k\}$ the subgraph of G which results from removing the edges $v_1w_1, \ldots, v_kw_k$.

For a single vertex (resp. edge), we will write $G - v$ (resp. $G - uv$) instead of $G - \{v\}$ (resp. $G - \{uv\}$).

Definition 2.1.5. The open neighbourhood of v denoted $N(v)$ is the set $\{u \in V(G) | uv \in E(G)\}$, and the closed neighbourhood of v is $N[v] = N(v) \cup \{v\}$. The *degree* of a vertex $v \in V(G)$ is $d_G(v) = |N(v)|$ (we write $d(v)$ if there is no ambiguity).

2.2 Special graphs

Definition 2.2.1. Let $V = \{v_1, v_2, \ldots, v_n\}$ be a set of vertices distinct from one another. The graph (V, E), where $E = \{v_1v_2, \ldots, v_{n-1}v_n\}$, is called a *path* and is denoted P_n.

Definition 2.2.2. Let $n \geq 3$ and V be the same set as in the previous definition. The graph (V, E), where $E = E(P_n) \cup \{v_1v_n\}$, is called a *cycle* and is denoted C_n.

Definition 2.2.3. A graph (V, E) of order n, where E contains all possible pairs of vertices in V is called a *complete graph* and denoted K_n. Note that $|E| = \frac{n(n-1)}{2}$.

Its complement, i.e., a graph (V, E) with $E = \emptyset$, is called an *edgeless graph* and is denoted E_n.

Definition 2.2.4. Let V be the same set as before. The graph (V, E), where $E = \{v_1v_2, v_1v_3, \ldots, v_1v_n\}$, is called a *star* and denoted S_n. The vertex v_1, which has degree $n - 1$ is called the *centre* of S_n.

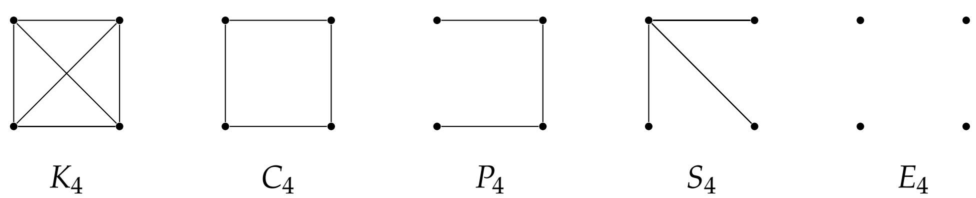


Figure 2.1: K_4, C_4, P_4, S_4, E_4.

Definition 2.2.5. A *line graph*, denoted $L(G)$, is a graph obtained from G such that $V(L(G)) = E(G)$ and there is an edge between two vertices of $L(G)$ if and only if the corresponding edges in G share a common endpoint.

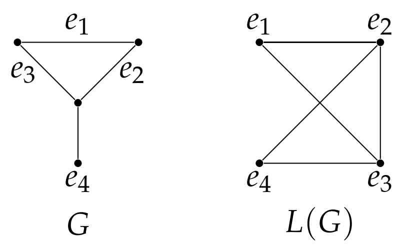


Figure 2.2: A graph G and its corresponding line graph $L(G)$.

Definition 2.2.6. A *subdivision graph*, denoted $S(G)$, is a graph obtained by inserting a new vertex of degree 2 on each edge of G.

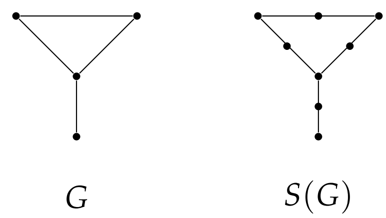


Figure 2.3: A graph G and its corresponding subdivision graph $S(G)$.

2.3 Connectivity, trees and forests

Definition 2.3.1. A graph G is said to be *connected* if and only if there is a path between any two vertices of G.

The *distance* between two vertices u and v, denoted $d(u,v)$, is the length of the shortest path between them.

Definition 2.3.2. An *acyclic* graph is a graph which does not contain any cycles. It is also called a *forest*.

Definition 2.3.3. A *tree* is a connected acyclic graph. The vertices whose degree is 1 are called *leaves*.

Let us now highlight some properties of trees that can be found in standard books on graph theory.

Proposition 2.3.4. *[19] A tree T satisfies the following properties:*

- *The number of edges in a tree of order n is $n-1$.*
- *There is a unique path between any two vertices of T.*

Definition 2.3.5. If we select a vertex v in a tree T to be its root, then T is called a *rooted tree*.

The height of a vertex $u \neq v$, denoted $h_T(u)$ ($h(u)$ if there is no ambiguity), is the distance of u and v, i. e. $d(u,v)$, and the height of the tree T denoted $h(T)$ is the maximum of $h_T(u)$ among all vertices.

Definition 2.3.6. A *starlike tree* $T(n_1, n_2, \ldots, n_k)$ is a tree composed of a root v, and the paths $P_1, P_2, \ldots, P_k$ of lengths $n_1, n_2, \ldots, n_k$ attached to v.

Definition 2.3.7. A *rooted forest* is a union of disjoint rooted trees.

Definition 2.3.8. Two rooted trees T and T' with roots r and r' are *rooted isomorphic*, denoted $T \approx_r T'$, if we can find a bijection $\ell : V(G) \to V(G')$ such that $uv \in E(G) \iff \ell(u)\ell(v) \in E(G')$ and $\ell(r) = r'$.

Example 2.3.9. Let us consider the trees T and T' rooted at r and r' respectively, see Figure 2.4. T and T' are isomorphic, but they are not rooted isomorphic.

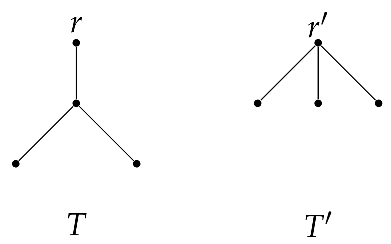


Figure 2.4: Isomorphic trees but not rooted isomorphic.

2.4 Graph parameters and graph polynomials

There are many different ways to obtain a graph polynomial. We will list some of them in this section.

2.4.1 Graph polynomials obtained from graph parameters

The first we are going to mention is to generate a graph polynomial from a graph parameter.

Definition 2.4.1. Let G be a graph. A subset A of $V(G)$ is called an *independent vertex subset* of G if $\{\{u,v\} : u,v \in A\} \cap E(G) = \emptyset$, i.e. if no two vertices in A are adjacent.

Definition 2.4.2. Let $\mathrm{i}(G,k)$ be the number of independent sets of size k of G. The *independence polynomial* ([27]) is defined as follows:

$$\mathrm{I}(G,x) = \sum_k \mathrm{i}(G,k)x^k.$$

Let v be a vertex of G and $N[v]$ its closed neighbourhood. The following result is straightforward from the definition of the independence polynomial.

Proposition 2.4.3 ([36]).

$$\mathrm{I}(G,x) = \mathrm{I}(G-v,x) + x\,\mathrm{I}(G-N[v],x), \tag{2.4.1}$$

where $N[v]$ is the closed neighbourhood of v as defined earlier.

Definition 2.4.4. Let G be a graph. A subset A of $E(G)$ is called a matching of G if the edges of A do not share common vertices.

Definition 2.4.5. Let $\mathrm{m}(G,k)$ be the number of matchings of size k in G.

The *matching polynomial* ([22]) is defined as:

$$\varphi(G,x) = \sum_{k\geq 0} (-1)^k \,\mathrm{m}(G,k)x^{|G|-2k}.$$

The *matching generating polynomial* is:

$$\mathrm{M}(G,x) = \sum_{k\geq 0} \mathrm{m}(G,k)x^k.$$

Let us mention some properties of matching polynomials found in [22]. These results are easily deduced from the definition of matching polynomials.

Proposition 2.4.6. *If G is a graph consisting of k components $G_1, G_2, \ldots, G_k$, then*

$$\mathrm{M}(G,x) = \prod_{i=1}^{k} \mathrm{M}(G_i,x).$$

Proposition 2.4.7. *If $e = uv$ is an edge of G, then*

$$\mathrm{M}(G, x) = \mathrm{M}(G - e, x) + x\,\mathrm{M}(G - u - v, x).$$

Proposition 2.4.8. *If v is a vertex of G, then*

$$\mathrm{M}(G, x) = \mathrm{M}(G - v, x) + x \sum_{u:uv \in E(G)} \mathrm{M}(G - v - u, x).$$

Similar polynomials can be obtained from other parameters such as subtrees ([3, 37]) and cliques ([36]).

2.4.2 Graph polynomials from matrices

Definition 2.4.9. Let G be an n-vertex graph, with $V = \{v_1, \ldots, v_n\}$. The *adjacency matrix* of G is the square matrix $A(G) = (a_{ij})_{1 \le i,j \le n}$, where:

$$a_{ij} = \begin{cases} 1 & \text{if} \quad v_i v_j \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

Definition 2.4.10. Let G be an n-vertex graph. The *characteristic polynomial* of G is:

$$\Phi(G, x) = det(xI_n - A(G)) = \sum_{k=0}^{n} a_k x^{n-k},$$

where I_n is the identity matrix of order n.

The coefficients of the characteristic polynomial can be determined by the famous Sachs theorem ([10]).

Theorem 2.4.11 (Sachs Theorem)**.** *Let G be a graph with characteristic polynomial $\Phi(G, x) = \sum_{k=0}^{n} a_k x^{n-k}$. Then for $k \ge 1$,*

$$a_k = \sum_{S \in L_k} (-1)^{w(S)} 2^{c(S)},$$

where L_k is the set of subgraphs of G with k vertices in which every component is either a K_2 or a cycle; $w(S)$ denotes the number of connected components of S and $c(S)$ is the number of cycles contained in S. Moreover, we have $a_0 = 1$.

Proposition 2.4.12. *[46] For the case of trees, the characteristic polynomial coincides with the matching polynomial.*

Definition 2.4.13. Let G be an n-vertex graph and $A(G)$ its adjacency matrix. The *Laplacian matrix* of G is $L(G) = A(G) - D(G)$, where $D(G)$ is the diagonal matrix whose diagonal entry d_{ii} corresponds to the degree of the i-th vertex v_i.

Definition 2.4.14. The *Laplacian polynomial* $\mathrm{L}(G)$ is the characteristic polynomial of the Laplacian matrix, i. e.,

$$\mathrm{L}(G, x) = det(xI_n - L(G)) = \sum_{k=0}^{n} C_k x^{n-k} = \sum_{k=0}^{n} (-1)^k c_k(G) x^{n-k}.$$

In 1967, Kel'mans ([40]) established a connection between the coefficients of the Laplacian polynomial and the structure of the graph. Let F be a spanning forest of p components denoted $F_1, \ldots, F_p$. We denote the number of vertices of each component F_i by $n(F_i)$. The product of the numbers $n(F_i)$, for $i = 1, \ldots, p$, is denoted $\gamma(F)$.

Theorem 2.4.15 (Kel'mans Theorem). *Let $C_0, C_1, \ldots, C_n$ be the coefficients of the Laplacian polynomial of a n-vertex graph G. Then,*

$$C_k = (-1)^k \sum_{F \in \mathrm{F}(G, n-k)} \gamma(F),$$

where $\mathrm{F}(G, p)$ is the set of all spanning forests of the graph G containing exactly p components.

Kel'mans Theorem shows already the connection between the coefficients of the Laplacian polynomial of a graph and its spanning forests. Considering that $\gamma(F)$ is the number of ways to assign roots to the forest F, $c_k(G)$ is the number of k-rooted spanning forests of G.

Proposition 2.4.16. *([9]) Let G be a graph and $W(G) = L(G) + I$. Then the determinant of $W(G)$ equals the total number of rooted spanning forests.*

Chapter 3

A Tutte-like polynomial for rooted trees

In this chapter, we are concerned with describing and investigating two-variable polynomials for rooted trees and for specific posets that are inspired by the Tutte polynomial. The basic concept for the Tutte polynomials can be traced back to [56, 57], in the context of colorings and flow problems in graphs. The Tutte polynomial has many properties and diverse applications, see for instance [4, 7]. In our context, we focus on the deletion-contraction property of the Tutte polynomial and its correspondence to the structure of the graph. Our polynomials share a similar property and are related to antichains and transversals, which are invariants for rooted trees. Counting problems on antichains have been explored in [41] and extremal questions are considered in [3]. On the other hand, transversals in trees have been investigated in [8, 24], with some applications in [21].

3.1 Introduction

For this section only, we will consider (general) graphs G with multiple edges and loops, because some of the constructions fail when restricted to simple graphs.

In 1912, Birkhoff [5] invented the chromatic polynomial to solve the map colorings problem.

Definition 3.1.1. The *chromatic polynomial* of a graph, denoted $\chi(G, x)$ is the number of ways to colour a graph G with x colours, where as usual an x-

colouring is a mapping $c : V(G) \to \{1, \ldots, x\}$ with $c(u) \neq c(v)$ if $uv \in E(G)$.

Example 3.1.2. Let us consider the chromatic polynomial of a star and a complete graph.

$$\chi(E_n, x) = x^n,$$
$$\chi(S_n, x) = x(x-1)^{n-1},$$
$$\chi(K_n, x) = x(x-1)\ldots(x-n+1).$$

Note that the *chromatic number* of G, which is the minimal number of colours needed to colour G, is the smallest positive integer κ with $\chi(G, \kappa) > 0$. An important fact about the chromatic polynomial is that it is indeed a polynomial. This is because for any coloring of G, the nonempty color classes constitute a partition of $V(G)$ where each part is an independent set. The total number of colorings is the sum of the colorings that give a certain partition for all possible partitions. Since $V(G)$ is a finite set, it has a finite number of partitions, so it is sufficient to show that the number of colorings for a single partition is a polynomial of x. If we fix a partition with p parts, by assigning a different color to each part, we get all the colorings belonging to the partition. We may pick the first color in x possible ways, the second in $x-1$ ways, etc. so there are $x(x-1)\ldots(x-p+1)$ colorings, which is obviously a polynomial.

Before going further, let us mention some special types of edges and some operations on graphs.

Definition 3.1.3. A *loop* is an edge whose end-vertices are the same and a *bridge* is an edge whose removal disconnects the component where it lies.

Definition 3.1.4. Let e be an edge. The *deletion* $G - e$ is the graph obtained from G by removing e. The *contraction* G/e is the graph that results after contracting e to a single vertex. Namely, the end-vertices of e are identified, all vertices adjacent to one of the two vertices involved in the contraction are adjacent to the contracted vertex in the resulting graph and all other adjacencies remain the same.

It is clear from the definitions that the chromatic polynomial satisfies the "deletion-contraction" property.

Proposition 3.1.5. *[4] Let e be an edge, which is not a loop of G. Then,*

$$\chi(G, x) = \chi(G - e, x) - \chi(G/e, x).$$

In 1954, Tutte [57] extended this result by considering two-variable polynomials. Let us give two equivalent definitions of the Tutte polynomial. The first one follows the deletion-contraction property of the chromatic polynomial with some boundary conditions.

Definition 3.1.6. Let G be a graph. The Tutte-polynomial $T(G;x,y)$ satisfies the following axioms:

- If $E(G) = \emptyset$, then $T(G;x,y) = 1$.
- If e is a bridge, then $T(G;x,y) = xT(G-e;x,y)$,
  if e is a loop, then $T(G;x,y) = yT(G-e;x,y)$.
- If e is neither a bridge nor a loop, then

$$T(G;x,y) = T(G-e;x,y) + T(G/e;x,y).$$

The second definition of the Tutte polynomial focuses on its relations to the rank of graphs. We denote by $k(G)$ the number of connected components of G.

Definition 3.1.7. Let G be a graph. Let A be a subset of $E(G)$, and identify A with the subgraph $G_A = (V(G), A)$. Thus all graphs G_A are spanning subgraphs of G. We define the *rank* of A by

$$r(A) = |V(G)| - k(G_A).$$

Remark 3.1.8. We easily notice that $0 \leq r(A) \leq |A|$ with

$$r(A) = 0 \iff A = \emptyset,$$
$$r(A) = |A| \iff G_A \text{ is a forest.}$$

Definition 3.1.9. Let G be a graph. The *rank polynomial* of G is defined as follows:

$$R(G;u,v) = \sum_{A \subseteq E(G)} u^{r(G)-r(A)} v^{|A|-r(A)}.$$

Theorem 3.1.10. *The Tutte polynomial $T(G;x,y)$ is uniquely given by*

$$T(G;x,y) = R(G;x-1,y-1).$$

For more details between the equivalence of the two definitions, we refer to [4].

Proposition 3.1.11. *The relation between the Tutte and rank polynomials leads us to the following evaluations. Let G be connected. Then*

$$T(G;1,1) = R(G;0,0) = \textit{number of spanning trees of } G,$$
$$T(G;2,1) = R(G;1,0) = \textit{number of spanning forests of } G,$$
$$T(G;1,2) = R(G;0,1) = \textit{number of connected spanning subgraphs of } G,$$
$$T(G;2,2) = R(G;1,1) = 2^{|E(G)|}.$$

3.2 A Tutte-like polynomial for rooted trees

The Tutte polynomial for trees is the same for any trees on n vertices since all edges in a tree are bridges. Furthermore, it is not defined for rooted trees. So, we want to consider a two-variable polynomial, which is meaningful for rooted trees and share similar properties as the Tutte polynomial. Let us first define some invariants for rooted trees.

Definition 3.2.1. An *antichain* is a set of vertices in which any two distinct vertices lie on different paths from the root to a leaf. A *maximal antichain* is an antichain that is not a proper subset of another antichain.

Let A be a subset of the vertices of T such that A is a *maximal antichain* in T. We define

$$\ell(A) = |\{a \in A; \quad \deg^+(a) = 0\}|,$$

where $\deg^+(a)$ is the outdegree of a. Note that we assume the direction of the edges is from the root towards a leaf. In other words $\ell(A)$ is the number of leaves contained in A. It is easy to see that $0 \leq \ell(A) \leq |A|$ with

$$\ell(A) = 0 \iff A \text{ does not contain any leaf},$$
$$\ell(A) = |A| \iff A \text{ is formed by all leaves of } T.$$

Let T_a be the subtree formed by a and all its successors, and $n(T_a) = |T_a| - 1$. We also define

$$c\ell(A) = \sum_{a \in A} n(T_a),$$

in particular $c\ell(A)$ is the number of vertices below the antichain A. We can again easily see that $0 \leq c\ell(A) \leq |T| - 1$ with

$$c\ell(A) = 0 \iff A \text{ is formed by all leaves of } T,$$
$$c\ell(A) = |T| - 1 \iff A \text{ only consists of the root}.$$

Now, we are able to define our polynomial in terms of maximal antichains.

Definition 3.2.2. Let $\mathcal{A}(T)$ be the set of all maximal antichains of T, then

$$\mathcal{P}(T;x,y) = \sum_{A\in\mathcal{A}(T)} x^{\ell(A)}\, y^{c\ell(A)}.$$

Our polynomial satisfies the following recursion:

Proposition 3.2.3. *Let T be a rooted tree and $T_1,\ldots,T_k$ its branches, then*

$$\mathcal{P}(T;x,y) = \begin{cases} x & \text{if } T \text{ has only one vertex,} \\ \prod_{i=1}^{k} \mathcal{P}(T_i;x,y) + y^{|T|-1} & \text{otherwise.} \end{cases}$$

Proof. We have to show that $\mathcal{P}(T;x,y)$ satisfies the recursion given in Proposition 3.2.3. It is straightforward that $\mathcal{P}(\bullet;x,y) = x$, since the only maximal antichain of the single-vertex tree $\bullet$ consists of the root, which has outdegree 0.

Now for $T \neq \bullet$, let $T_1,\ldots,T_k$ be the branches attached to the root. We can see that

$$\mathcal{A}(T) = \{A_1 \cup A_2 \cup \cdots \cup A_k; A_i \in \mathcal{A}(T_i) \text{ for } 1 \leq i \leq k\} \cup \{\{r\}\}.$$

Thus,

$$\begin{aligned} \mathcal{P}(T;x,y) &= \sum_{A\in\mathcal{A}(T)} x^{\ell(A)}\, y^{c\ell(A)} \\ &= \prod_{i=1}^{k} \left(\sum_{A_i\in\mathcal{A}(T_i)} x^{\ell(A)}\, y^{c\ell(A)} \right) + \sum_{A=\{r\}} x^{\ell(A)}\, y^{c\ell(A)} \\ &= \prod_{i=1}^{k} \mathcal{P}(T_i;x,y) + y^{|T|-1}. \end{aligned}$$

■

Definition and Proposition 3.2.3 uniquely determine our polynomial $\mathcal{P}$. Let us consider some examples.

Example 3.2.4.

$$\mathcal{P}(S_n;x,y) = x^{n-1} + y^{n-1},$$

where S_n is the star on n vertices rooted at its centre.

$$\mathcal{P}(P_n;x,y) = x + y + y^2 + \cdots + y^{n-1},$$

where P_n is the path on n vertices rooted at one of its endpoints.

Now, we want to investigate if our polynomials can be written using an appropriate deletion-contraction recursion. Let us define the following operations on rooted trees.

Definition 3.2.5. Let e be an edge incident to the root and to a vertex u_i and T_i be the branch attached to u_i. The *contraction* T/e is the tree that results after contracting e to the root. That is, the root and u_i are merged. The *deletion* $T - T_i$ is the tree obtained from removing the branch T_i.

Definition 3.2.6. A pendant edge is an edge which is incident to a leaf. We call an edge a "bridge" if it disconnects the root from all of its successors.

Now, let us characterize our polynomial using a "deletion-contraction" procedure as with the Tutte polynomial.

Proposition 3.2.7. *Let e be any edge incident to the root r and a vertex u_i. We have*

1. $\mathcal{P}(T;x,y) = \mathcal{P}(T/e;x,y) + y^{|T|-1}$ *if e is a bridge,*
2. $\mathcal{P}(T;x,y) = x\mathcal{P}(T/e;x,y) - xy^{|T|-2} + y^{|T|-1}$ *if e is a pendant edge,*
3. $\mathcal{P}(T;x,y) = \mathcal{P}(T/e;x,y) + y^{|T_i|-1}\mathcal{P}(T-T_i;x,y) - 2y^{|T|-2} + y^{|T|-1}$ *if e is not a bridge, nor a pendant edge, and e is attached to a branch T_i.*

Proof. 1. If e is a bridge attached to the branch T_1, then

$$\mathcal{P}(T;x,y) = \mathcal{P}(T_1;x,y) + y^{|T|-1} = \mathcal{P}(T/e;x,y) + y^{|T|-1}.$$

2. If e is a pendant edge attached to the single-vertex branch T_1, then

$$\begin{aligned}
\mathcal{P}(T;x,y) - y^{|T|-1} &= \prod_{i=1}^{k} \mathcal{P}(T_i;x,y) \\
&= \mathcal{P}(T_1;x,y)\prod_{i=2}^{k} \mathcal{P}(T_i;x,y) = x\prod_{i=2}^{k} \mathcal{P}(T_i;x,y) \\
&= x(\mathcal{P}(T/e;x,y) - y^{|T|-2}) \\
&= x\mathcal{P}(T/e;x,y) - xy^{|T|-2}.
\end{aligned}$$

3. Let e be an edge incident to the root and u_1 not a bridge nor a pendant edge and attached to the branch T_1. Denote the branches attached to u_1 by $B_1, B_2, \ldots, B_\ell$.

$$
\begin{aligned}
\mathcal{P}(T;x,y) - y^{|T|-1} &= \prod_{i=1}^{k} \mathcal{P}(T_i;x,y) = \mathcal{P}(T_1;x,y)\prod_{i=2}^{k}\mathcal{P}(T_i;x,y) \\
&= \left(\prod_{j=1}^{\ell}\mathcal{P}(B_j;x,y) + y^{|T_1|-1}\right)\prod_{i=2}^{k}\mathcal{P}(T_i;x,y) \\
&= \prod_{j=1}^{\ell}\mathcal{P}(B_j;x,y)\prod_{i=2}^{k}\mathcal{P}(T_i;x,y) + y^{|T_1|-1}\prod_{i=2}^{k}\mathcal{P}(T_i;x,y) \\
&= \mathcal{P}(T/e;x,y) - y^{|T|-2} \\
&\quad + y^{|T_1|-1}\left(\mathcal{P}(T-T_1;x,y) - y^{|T|-|T_1|-1}\right) \\
&= \mathcal{P}(T/e;x,y) + y^{|T_1|-1}\mathcal{P}(T-T_1;x,y) - 2y^{|T|-2}.
\end{aligned}
$$

■

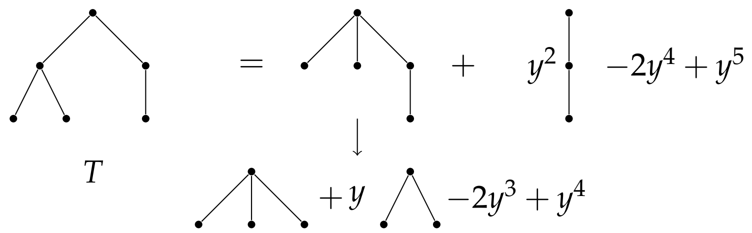


Figure 3.1: Computing $\mathcal{P}(T;x,y)$ using deletion-contraction recursion.

Example 3.2.8. As we can see from Figure 3.1, we get

$$
\begin{aligned}
\mathcal{P}(T;x,y) &= (x^3+y^3) + y(x^2+y^2) - 2y^3 + y^4 + y^2(x+y+y^2) - 2y^4 + y^5 \\
&= x^3 + y^2x + x^2y + y^3 + y^5.
\end{aligned}
$$

Definition 3.2.9. ([8]) A *transversal* in a rooted tree is a set of vertices that meets every path from the root to a leaf.

Proposition 3.2.10. *We have the following evaluations:*

$$
\begin{aligned}
\mathcal{P}(T;1,1) &= \textit{number of maximal antichains of } T, \\
\mathcal{P}(T;x,0) &= x^{\textit{number of leaves in } T}, \\
\mathcal{P}(T;0,1) &= \textit{number of maximal antichains with no leaves}, \\
\mathcal{P}(T;2,1) &= \textit{number of antichains of } T, \\
\mathcal{P}(T;1,2) &= \textit{number of transversals of } T, \\
\mathcal{P}(T;2,2) &= 2^{|T|}.
\end{aligned}
$$

Proof. The first three evaluations are straightforward from the definition of $\mathcal{P}(T;x,y)$.

The fourth evaluation comes from the fact that every antichain can be obtained uniquely from a maximal antichain by removing a subset (possibly empty) of the leaves contained in it.

The fifth evaluation is due to the fact that a transversal can be formed uniquely from a maximal antichain by including a subset (possibly empty) of the successors. From a recursive perspective, the number of transversals of a rooted tree T is the product of the number of transversals of all the branches of T plus the number of transversals which contain the root. Since any subsets of $|T|$ containing the root is a transversal, the later corresponds to $2^{|T|-1}$. Hence, the recursion in Proposition 3.2.3 for $x = 1$ and $y = 2$ corresponds to the recursion of the number of transversals.

The last evaluation counts the number of all subsets of any size among all the vertices, which is exactly $2^{|T|}$. The number of subsets of a tree T is the product of the number of subsets of all the branches of T plus the number of subsets which contain the root. That is $2^{\sum_{i=1}^{k}|T_i|} + 2^{|T|-1} = 2^{|T|}$. ■

Remark 3.2.11. If we fix one of the variables in $\mathcal{P}(T;x,y)$, we can find non-isomorphic rooted trees having the same $\mathcal{P}$.

Example 3.2.12. Let us consider the trees in Figure 3.2. We have the following evaluations:

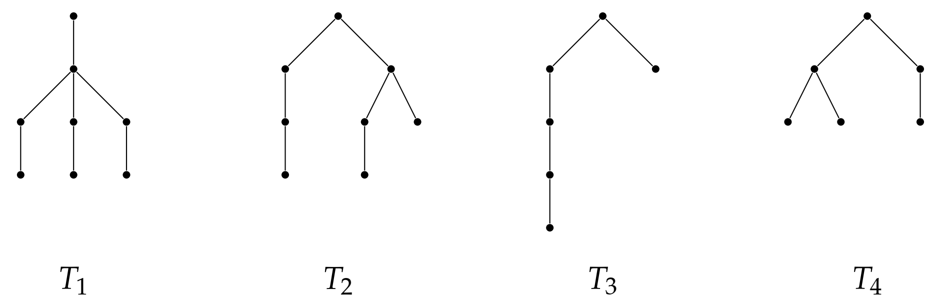


Figure 3.2: Non rooted isomorphic trees.

$$\mathcal{P}(T_1;x,1) = \mathcal{P}(T_2;x,1) = x^3 + 3x^2 + 3x + 3,$$
$$\mathcal{P}(T_3;1,y) = \mathcal{P}(T_4;1,y) = y^5 + y^3 + y^2 + y + 1.$$

However, note that

$$\begin{aligned}
\mathcal{P}(T_1;x,y) &= y^7+y^6+y^3+3y^2x+3yx^2+x^3 \\
&\neq y^7+y^5+y^4+2y^3x+y^2x^2+y^2x+2yx^2+x^3=\mathcal{P}(T_2;x,y), \\
\mathcal{P}(T_3;x,y) &= y^5+y^3x+y^2x+yx+x^2 \\
&\neq y^5+y^3+y^2x+yx^2+x^3=\mathcal{P}(T_4;x,y).
\end{aligned}$$

These observations lead to the following conjecture:

Conjecture 3.2.13. If $\mathcal{P}(T;x,y)=\mathcal{P}(T';x,y)$, then T and T' are isomorphic rooted trees.

3.3 A Tutte-like polynomial for posets

In this section, we consider specific posets and we generalise the results obtained for our Tutte-like polynomial for rooted trees to those posets.

Definition 3.3.1. Let a V-poset be a poset that can be generated by the following three operations:

1. a disjoint union,
2. adding a new greatest element,
3. adding a new least element.

Note that the empty poset is considered as a V-poset.

Let $\mathcal{V}$ be the set of all V-posets.

Definition 3.3.2. We define a Tutte-like polynomial $\mathcal{P}$ for $P \in \mathcal{V}$ as follows:

$$\begin{aligned}
\mathcal{P}(\emptyset;x,y) &= 1, \\
\mathcal{P}(\bullet;x,y) &= x, \\
\mathcal{P}(\cup_i P_i;x,y) &= \prod_i \mathcal{P}(P_i;x,y), \quad \text{where } \cup_i P_i \text{ is a disjoint union,} \\
\mathcal{P}(P\cup g;x,y) &= \mathcal{P}(P\cup \ell;x,y)=\mathcal{P}(P;x,y)+y^{|P|},
\end{aligned}$$

where g and ℓ are respectively a greatest and a least element.

Example 3.3.3. Let us compute the $\mathcal{P}$-polynomial of the poset P given in Figure 3.3.

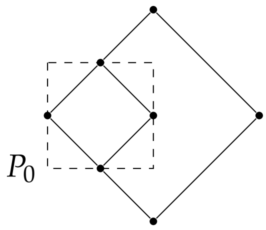


Figure 3.3: A poset P

$$\mathcal{P}(P;x,y) = x\mathcal{P}(P_0;x,y) + y^5 + y^6 = x(x^2 + y^2 + y^3) + y^5 + y^6.$$

Definition 3.3.4. An *antichain* is a subset of a poset in which any two distinct elements are incomparable. A *maximal antichain* is one that is not a proper subset of any other antichain. A *transversal* is a set of elements in a poset that intersects every maximal chain (maximal totally ordered sub-poset).

Proposition 3.3.5. *Let P be a V-poset. The following evaluations hold:*

$$\begin{aligned}
\mathcal{P}(P;1,1) &= \textit{number of maximal antichains in } P,\\
\mathcal{P}(P;2,1) &= \textit{number of antichains in } P \textit{ (including } \emptyset),\\
\mathcal{P}(P;1,2) &= \textit{number of transversals in } P,\\
\mathcal{P}(P;2,2) &= 2^{|P|}.
\end{aligned}$$

Proof. These evaluations are straightforward from the recursion in Definition 3.3.2. ∎

Now, we are interested in finding out more about the set of all V-posets. Let $V(x)$ be the generating function of $\mathcal{V}$, i.e.

$$V(x) = \sum_n v_n x^n,$$

where v_n is the number of V-posets of size n. For convenience, we set $v_0 = 1$.

Let $\mathcal{Q}$ be the set of "connected" V-posets i.e, posets which have a least or greatest element, and denote its generating function by $Q(x)$. Following Definition 3.3.1, an element of $\mathcal{Q}$ is formed by adding a least or greatest element to a V-poset. However, the cases that there are both a least and a greatest element and the one element V-poset are counted twice, so we subtract these cases. This reasoning can be translated to the following equation:

$$Q(x) = (2x - x^2)V(x) - x.$$

Furthermore, every element of $\mathcal{V}$ is a multiset of elements of $\mathcal{Q}$, thus by [23, Theorem I.1]:

$$\begin{aligned} V(x) &= \exp\left(\sum_{m\geq 1} \frac{Q(x^m)}{m}\right) \\ &= \exp\left(\sum_{m\geq 1} \frac{(2x^m - x^{2m})V(x^m) - x^m}{m}\right) \\ &= \exp\left(-\log\frac{1}{1-x}\right)\exp\left(\sum_{m\geq 1} \frac{(2x^m - x^{2m})V(x^m)}{m}\right) \\ &= (1-x)\exp\left(\sum_{m\geq 1} \frac{(2x^m - x^{2m})V(x^m)}{m}\right). \end{aligned}$$

This gives,

$$V(x) = 1 + x + 2x^2 + 5x^3 + 14x^4 + 40x^5 + 121x^6 + 373x^7 + 1184x^8 + \cdots$$

For example, we can see that there are 121 V-posets with 6 elements. Set $W(x) = Q(x) + x = x(2-x)V(x)$, then

$$W(x) = x(1-x)(2-x)\exp\left(\sum_{m\geq 2} \frac{W(x^m)}{m}\right)\exp\left(W(x)\right),$$

so

$$W(x) = T\left(x(1-x)(2-x)\exp\left(\sum_{m\geq 2} \frac{W(x^m)}{m}\right)\right),$$

where T is the tree function given implicitly by $T = x\exp(T)$. For more information about the tree function, we refer to [49].

Furthermore, if $W(x) = \sum_{n\geq 1} w_n x^n$, then we have for $0 \leq x < 1$:

$$\sum_{m\geq 2}\frac{W(x^m)}{m} = \sum_{m\geq 2}\sum_{n\geq 1}\frac{w_n\, x^{mn}}{m} \leq \sum_{n\geq 1} w_n \sum_{m\geq 2} x^{mn}$$

$$= \sum_{n\geq 1} w_n \frac{x^{2n}}{1-x^n} \leq \frac{1}{1-x}\sum_{n\geq 1} w_n x^{2n} = \tag{3.3.1}$$

$$= \frac{1}{1-x}W(x^2). \tag{3.3.2}$$

Now, write

$$R(x) = x(1-x)(2-x)\exp\left(\sum_{m\geq 2}\frac{W(x^m)}{m}\right).$$

From (3.3.2), we see that $R(x)$ has greater radius of convergence than $W(x)$; since T only has a branch cut singularity at $1/e$ with expansion

$$T(x) = 1 - \sqrt{2(1-ex)} + \mathcal{O}(1-ex),$$

the function W becomes singular when $R(x) = \frac{1}{e}$, which is at $\rho \approx 0.263436$. We have an expansion of $R(x)$ as follows:

$$R(x) = R(\rho) + R'(\rho)(x-\rho) + \mathcal{O}((x-\rho)^2),$$

so

$$W(x) = T(R(x)) = 1 - \sqrt{2e\rho R'(\rho)}\left(1-\frac{x}{\rho}\right)^{1/2} + \mathcal{O}\left(1-\frac{x}{\rho}\right)$$

and therefore

$$V(x) = \frac{1}{2x-x^2}W(x) = \frac{1}{2\rho-\rho^2} - \frac{\sqrt{2e\rho R'(\rho)}}{2\rho-\rho^2}\left(1-\frac{x}{\rho}\right)^{1/2} + \mathcal{O}\left(1-\frac{x}{\rho}\right)$$

Now singularity analysis [23, Theorem VI.4] gives us the following theorem:

Theorem 3.3.6. *The number of V-posets of size n is given by the following asymptotic formula when n tends to infinity:*

$$v_n \sim \frac{\sqrt{2e\rho R'(\rho)}}{2\sqrt{\pi}(2\rho-\rho^2)}n^{-3/2}\rho^{-n} = \frac{\sqrt{eR'(\rho)}}{\sqrt{2\pi\rho}(2-\rho)}n^{-3/2}\rho^{-n},$$

where $\frac{\sqrt{eR'(\rho)}}{\sqrt{2\pi\rho}(2-\rho)} \approx 0.726213$, *and* $\frac{1}{\rho} \approx 3.79599$.

Chapter 4

The average size of independent sets in a graph

In 1983, Jamison [37] investigated the average order of subtrees of a tree. Namely, this quantity is the logarithmic derivative of the generating function of subtrees of T at 1, i.e., $M_T = \frac{\Phi'_T(1)}{\Phi_T(1)}$. He found that the average order of subtrees of an n-vertex tree is at least $(n+2)/3$ (the equality holds for the path), and proposed several questions on this invariant. Further, in 1984 [38], he established the monotonicity of this mean. Later in 2010, Vince and Wang [58] showed that the average order lies between 1/2 and 3/4 for trees without vertices of degree 2, answering one of the conjectures of Jamison [37]. The study of the average order of subtrees attracted more and more attention, we may refer to [31] and [62]. In this chapter, we consider the average size of independent sets in a graph, inspired from the average order of subtrees, taking independent sets instead of subtrees. Different authors have already studied bounds on this invariant for specific graphs, see [12] and [13]. Here, we characterize extremal graphs for this quantity. Extremal problems regarding the number of independent sets of a graph have been extensively studied. See for example, the case for general graphs with additional restrictions [43, 68, 76], the class of trees [1, 33, 42, 47, 51, 52], unicyclic graphs [16, 50, 64], bicyclic graphs [17, 18, 54] and many more [61].

4.1 The average size of independent sets in a graph

4.1.1 Preliminaries

Let G be a graph, and let $\mathrm{i}(G,k)$ be the number of independent sets of size k. Let $\mathrm{I}(G,x)$ be the independence polynomial of G. Then the total number of independent subsets of G is

$$\mathrm{I}(G,1) = \sum_k \mathrm{i}(G,k).$$

The first derivative of I for $x = 1$ is

$$\mathrm{I}'(G,1) = \sum_k k\,\mathrm{i}(G,k),$$

so that the average size of the independent vertex subsets in G is

$$\mathrm{avi}(G) = \frac{\mathrm{I}'(G,1)}{\mathrm{I}(G,1)}.$$

For ease of notation, we will write $\mathrm{I}(G)$ instead of $\mathrm{I}(G,1)$, as well as $\mathrm{T}(G)$ instead of $\mathrm{I}'(G,1)$.

For example, for the n-vertex edgeless graph E_n and star S_n we have $\mathrm{I}(E_n) = 2^n$, $\mathrm{I}(S_n) = 2^{n-1} + 1$,

$$\mathrm{T}(E_n) = \sum_{k=0}^{n} \binom{n}{k} k = n2^{n-1}, \quad \mathrm{T}(S_n) = (n-1)2^{n-2} + 1$$

and hence

$$\mathrm{avi}(E_n) = \frac{n}{2}, \quad \mathrm{avi}(S_n) = \frac{n-1}{2} + \frac{3-n}{2^n+2}.$$

Proposition 4.1.1. *Let v be a vertex of G and $N[v]$ its closed neighbourhood. We have*

$$\mathrm{I}(G) = \mathrm{I}(G-v) + \mathrm{I}(G-N[v]), \tag{4.1.1}$$

$$\mathrm{T}(G) = \mathrm{T}(G-v) + \mathrm{T}(G-N[v]) + \mathrm{I}(G-N[v]). \tag{4.1.2}$$

Proof. We obtain the desired result by summing up the cardinality of independent sets not containing v first and then that of those which contain v. ∎

Thus, we get the following recursion for the average size of independent sets:

Proposition 4.1.2.

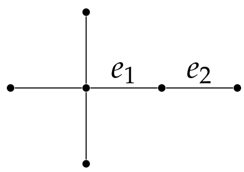
$$\begin{aligned}\operatorname{avi}(G) &= \frac{\mathrm{T}(G-v)+\mathrm{T}(G-N[v])+\mathrm{I}(G-N[v])}{\mathrm{I}(G-v)+\mathrm{I}(G-N[v])}\\ &= \frac{\operatorname{avi}(G-v)\,\mathrm{I}(G-v)+(\operatorname{avi}(G-N[v])+1)\,\mathrm{I}(G-N[v])}{\mathrm{I}(G-v)+\mathrm{I}(G-N[v])}.\end{aligned}$$

4.1.2 Vertex or edge removal

Unlike I, avi is not always increasing under addition of a vertex (resp. decreasing under addition of an edge) to the graph. If v and u are respectively a leaf and the centre of S_4, then we have

$$\begin{aligned}\operatorname{avi}(S_4-v) &= \operatorname{avi}(S_3) = 1 < \frac{13}{9} = \operatorname{avi}(S_4),\\ \operatorname{avi}(S_4-u) &= \operatorname{avi}(E_3) = \frac{3}{2} > \operatorname{avi}(S_4).\end{aligned}$$

Considering the graph



T

we get

$$\begin{aligned}\operatorname{avi}(T-e_1) &= \frac{13}{9}+\frac{2}{3} = \frac{19}{9} < \frac{55}{26} = \operatorname{avi}(T),\\ \operatorname{avi}(T-e_2) &= \frac{33}{17}+\frac{1}{2} = \frac{83}{34} > \operatorname{avi}(T).\end{aligned}$$

Clearly, the centre u is the only vertex of S_4 which satisfies $\operatorname{avi}(S_4-u) > \operatorname{avi}(S_4)$. In general, for any given nonempty graph G, there is always a vertex w in G such that its removal reduces avi. This will follow as application of the following theorem:

Theorem 4.1.3. *Let X be a nonempty finite set, and $\mathcal{P}(X)$ its powerset. For any $\mathcal{A} \subseteq \mathcal{P}(X)$, we define*

$$av(\mathcal{A}) = \frac{1}{|\mathcal{A}|}\sum_{A\in\mathcal{A}} |A|.$$

Let $\mathcal{B} \subseteq \mathcal{P}(X)$, such that the cardinalities of the elements of $\mathcal{B}$ are not all the same and for every $x \in X$ there exists $B \in \mathcal{B}$ with $x \in B$. Then there exists $x_0 \in X$ such that

$$av(\mathcal{B}) > av\big(\mathcal{B} \cap \mathcal{P}(X - \{x_0\})\big).$$

Proof. It is convenient to abbreviate

$$n_k(\mathcal{A}) = \big|A \in \mathcal{A} : |A| = k\big| \text{ and } S(\mathcal{A}) = \sum_{A \in \mathcal{A}} |A| = \sum_{k \geq 0} k \cdot n_k(\mathcal{A}).$$

We prove that

$$av(\mathcal{B}) > \frac{\sum_{x \in X} S(\mathcal{B} \cap \mathcal{P}(X - \{x\}))}{\sum_{x \in X} |\mathcal{B} \cap \mathcal{P}(X - \{x\})|},$$

and the claim of the theorem follows trivially, because

$$\frac{\sum_{x \in X} S(\mathcal{B} \cap \mathcal{P}(X - \{x\}))}{\sum_{x \in X} |\mathcal{B} \cap \mathcal{P}(X - \{x\})|} \geq \min_{x \in X} \frac{S(\mathcal{B} \cap \mathcal{P}(X - \{x\}))}{|\mathcal{B} \cap \mathcal{P}(X - \{x\})|}.$$

In

$$\sum_{x \in X} S(\mathcal{B} \cap \mathcal{P}(X - \{x\})) = \sum_{x \in X} \sum_{k \geq 0} k \cdot n_k(\mathcal{B} \cap \mathcal{P}(X - \{x\})),$$

the size of each $B \in \mathcal{B}$ contributes $|X| - |B|$ times. Hence

$$\begin{aligned}
&\sum_{x \in X} S(\mathcal{B} \cap \mathcal{P}(X - \{x\})) \\
&= \sum_{k \geq 0} (|X| - k) k \cdot n_k(\mathcal{B}) = |X| S(\mathcal{B}) - \sum_{k \geq 0} k^2 n_k(\mathcal{B}) \\
&= |X| av(\mathcal{B}) |\mathcal{B}| - \sum_{k \geq 0} k^2 n_k(\mathcal{B}).
\end{aligned}$$

Similarly,

$$\begin{aligned}
\sum_{x \in X} |\mathcal{B} \cap \mathcal{P}(X - \{x\})| &= \sum_{x \in X} \sum_{k \geq 0} n_k(\mathcal{B} \cap \mathcal{P}(X - \{x\})) \\
&= \sum_{x \in X} \sum_{k \geq 0} (|X| - k) n_k(\mathcal{B}) \\
&= |X||\mathcal{B}| - S(\mathcal{B}).
\end{aligned}$$

Note that by the Cauchy-Schwarz inequality, we obtain

$$\begin{aligned}
S(\mathcal{B})^2 = \left(\sum_{k \geq 0} k \cdot n_k(\mathcal{B}) \right)^2 &= \left(\sum_{k \geq 0} k \sqrt{n_k(\mathcal{B})} \sqrt{n_k(\mathcal{B})} \right)^2 \\
\leq \sum_{k \geq 0} (k \sqrt{n_k(\mathcal{B})})^2 \sum_{k \geq 0} (\sqrt{n_k(\mathcal{B})})^2 \\
= \sum_{k \geq 0} k^2 n_k(\mathcal{B}) \sum_{k \geq 0} n_k(\mathcal{B}) = |\mathcal{B}| \sum_{k \geq 0} k^2 n_k(\mathcal{B}),
\end{aligned}$$

and the equality holds if and only if there is only one k such that $n_k(\mathcal{B}) \neq 0$, which means all the elements of $\mathcal{B}$ have the same size. Since this is ruled out by our assumptions, we have

$$av(\mathcal{B})S(\mathcal{B}) < \sum_{k\geq 0} k^2 n_k(\mathcal{B}).$$

Therefore we get

$$\begin{aligned}\frac{\sum_{x\in X} S(\mathcal{B}\cap\mathcal{P}(X-\{x\}))}{\sum_{x\in X}|\mathcal{B}\cap\mathcal{P}(X-\{x\})|} &= \frac{|X|av(\mathcal{B})|\mathcal{B}| - \sum_{k\geq 0} k^2 n_k(\mathcal{B})}{|X||\mathcal{B}| - S(\mathcal{B})} \\ &< \frac{|X|av(\mathcal{B})|\mathcal{B}| - av(\mathcal{B})S(\mathcal{B})}{|X||\mathcal{B}| - S(\mathcal{B})} = av(\mathcal{B}).\end{aligned}$$

■

Corollary 4.1.4. *If G is a nonempty graph, then there exists a vertex v in G such that*

$$\text{avi}(G - v) < \text{avi}(G).$$

Proof. Apply Theorem 4.1.3, with $\mathcal{B}$ being the set of independent vertex subsets of G. ■

We have seen that there is always a vertex in a graph which removal decreases the average size of independent sets avi. However, the dual statement for edge removal does not hold, namely there is not always an edge whose removal increases avi. As a counterexample, we can consider S_6: for any edge e in S_6 we have

$$\text{avi}(S_6) = \frac{27}{11} > \frac{83}{34} = \text{avi}(S_6 - e).$$

So, every edge removal in S_6 decreases avi.

Despite this the edgeless graphs and the complete graphs are still extremal graphs:

Theorem 4.1.5. *For any n-vertex graph G which is not the edgeless graph E_n nor the complete graph K_n, $\frac{n}{n+1} = \text{avi}(K_n) < \text{avi}(G) < \text{avi}(E_n) = \frac{n}{2}$.*

Proof. The first inequality is straightforward from the fact that the only independent sets of K_n are n independent sets of size 1 and the empty set. We prove the second inequality by induction. For $n = 1$, there is no possible graph different from E_n, so there is nothing to prove. Now, assume that the inequality is true for any $n \leq k$, for some $k \geq 1$. Let G be an $(k+1)$-vertex graph which is not edgeless and not complete. Let $v \in V(G)$ be a vertex such that $\deg(v) \geq 1$. We have

$$\mathrm{avi}(G) = \frac{\mathrm{T}(G-v) + \mathrm{T}(G-N[v]) + \mathrm{I}(G-N[v])}{\mathrm{I}(G-v) + \mathrm{I}(G-N[v])}.$$

Using the induction hypothesis, we obtain

$$\begin{aligned}\mathrm{avi}(G) &\leq \frac{\frac{k}{2}\,\mathrm{I}(G-v) + (\frac{k-1}{2}+1)(\mathrm{I}(G-N[v]))}{\mathrm{I}(G-v) + \mathrm{I}(G-N[v])} \\ &= \frac{k}{2} + \frac{\frac{1}{2}\,\mathrm{I}(G-N[v])}{\mathrm{I}(G-v) + \mathrm{I}(G-N[v])} \\ &< \frac{k}{2} + \frac{1}{2} = \frac{k+1}{2} = \mathrm{avi}(E_{k+1}).\end{aligned}$$

■

4.1.3 The case of trees

Let us first consider the problem on the maximization of the average size of independent sets among all n-vertex trees.

Theorem 4.1.6. *For any n-vertex tree T, $\mathrm{avi}(S_n) \geq \mathrm{avi}(T)$.*

Proof. In the cases where $n = 1, 2, 3$, we must have $T = S_n$, and thus the claim holds.

Assume the inequality holds for all $n \leq k$, for some $k \geq 3$. Now suppose that $T \neq S_n$ is a tree with $n = k+1$ vertices. Let $v \in V(T)$ be a leaf of T. Then $T - v$ is still a tree, $\mathrm{I}(T-v) - \mathrm{I}(T-N[v]) > 1$, and $\mathrm{I}(T-v) \leq \mathrm{I}(S_{n-1})$ (see [52]).

$$\frac{\mathrm{I}(T-N[v])}{\mathrm{I}(T-v)} = 1 - \frac{\mathrm{I}(T-v) - \mathrm{I}(T-N[v])}{\mathrm{I}(T-v)} < 1 - \frac{1}{\mathrm{I}(T-v)} \leq 1 - \frac{1}{2^{n-2}+1}. \tag{4.1.3}$$

Using Theorem 4.1.5, we have

$$\begin{aligned}\mathrm{avi}(T) &= \frac{\mathrm{avi}(T-v)\,\mathrm{I}(T-v) + (\mathrm{avi}(T-N[v])+1)\,\mathrm{I}(T-N[v])}{\mathrm{I}(T-v) + \mathrm{I}(T-N[v])} \\ &\leq \frac{\mathrm{avi}(S_{n-1})\,\mathrm{I}(T-v)/\,\mathrm{I}(T-N[v]) + \frac{n-2}{2} + 1}{\mathrm{I}(T-v)/\,\mathrm{I}(T-N[v]) + 1}.\end{aligned}$$

Since $\operatorname{avi}(S_{n-1}) < \frac{n-2}{2}+1$, $\frac{\operatorname{avi}(S_{n-1})x+\frac{n-2}{2}+1}{x+1}$ is decreasing for $x \geq 0$, and using Equation (4.1.3), we obtain:

$$\operatorname{avi}(T) < \frac{\operatorname{avi}(S_{n-1})(2^{n-2}+1)/2^{n-2}+\frac{n-2}{2}+1}{(2^{n-2}+1)/2^{n-2}+1} = \operatorname{avi}(S_n).$$

■

To prove that the path has the minimum average size of independent sets requires more techniques. Let us first find an explicit formula of the average size of independent sets of a path.

Lemma 4.1.7. *The average size of independent sets of the n-vertex path P_n is*

$$\operatorname{avi}(P_n) = \frac{5-\sqrt{5}}{10}n + \frac{3-\sqrt{5}}{5} - \frac{n+2}{\sqrt{5}((-\phi^2)^{n+2}-1)}, \tag{4.1.4}$$

where $\phi = \frac{\sqrt{5}+1}{2}$ is the golden ratio. In particular,

(a) $\lim_{n\to\infty} \operatorname{avi}(P_n) - \frac{5-\sqrt{5}}{10}n = \frac{3-\sqrt{5}}{5}$,

(b) $\operatorname{avi}(P_n) \geq \frac{5-\sqrt{5}}{10}n + \frac{1}{\sqrt{5}} - \frac{1}{3}$, *with equality only for $n = 2$. For all positive integers $n \neq 2$, we even have* $\operatorname{avi}(P_n) \geq \frac{5-\sqrt{5}}{10}n + \frac{2}{\sqrt{5}} - \frac{3}{4}$.

Proof. It is well known that the number of independent sets of P_n is the Fibonacci number $F_{n+2} = \frac{1}{\sqrt{5}}(\phi^{n+2} - (-\phi)^{-n-2})$ (see [52]). The total number of vertices $\mathrm{T}(P_n)$ in all independent sets of P_n is determined by the recursion

$$\mathrm{T}(P_n) = \mathrm{T}(P_{n-1}) + \mathrm{T}(P_{n-2}) + \mathrm{I}(P_{n-2})$$

and the initial values $\mathrm{T}(P_1) = 1$ and $\mathrm{T}(P_2) = 2$. The formula (4.1.4) for the quotient $\operatorname{avi}(P_n) = \mathrm{T}(P_n)/\,\mathrm{I}(P_n)$ follows immediately, as does the limit in (a).

Now we show that the absolute value of the error term is decreasing: for $n \geq 2$, we have

$$\begin{aligned}
\left| \frac{\frac{n+2}{\sqrt{5}((-\phi^2)^{n+2}-1)}}{\frac{n+1}{\sqrt{5}((-\phi^2)^{n+1}-1)}} \right| &\leq \left(1+\frac{1}{n+1}\right)\cdot\frac{\phi^{2(n+1)}+1}{\phi^{2(n+2)}-1} \\
&= \phi^{-2}\left(1+\frac{1}{n+1}\right)\cdot\frac{\phi^{-2(n+1)}+1}{1-\phi^{-2(n+2)}} \\
&\leq \phi^{-2}\cdot\frac{4}{3}\cdot\frac{\phi^{-6}+1}{1-\phi^{-8}} = \frac{4(\sqrt{5}-1)}{9} < 1.
\end{aligned}$$

Therefore, the difference

$$\left| \operatorname{avi}(P_n) - \frac{5-\sqrt{5}}{10}n - \frac{3-\sqrt{5}}{5} \right|$$

is decreasing in n. Moreover, note that the sign of $\frac{n+2}{\sqrt{5}((-\phi^2)^{n+2}-1)}$ alternates, so that $\operatorname{avi}(P_n)$ is alternatingly greater and less than $\frac{5-\sqrt{5}}{10}n + \frac{3-\sqrt{5}}{5}$. It follows that the minimum of the difference $\operatorname{avi}(P_n) - \frac{5-\sqrt{5}}{10}n$ is attained for $n = 2$. Among all $n \neq 2$, the minimum occurs when $n = 4$. The values of $\operatorname{avi}(P_n)$ are easily calculated in both cases, and the two inequalities in (b) follow. ∎

For ease of notation, we set $a = \frac{5-\sqrt{5}}{10} \approx 0.27639320$ and $c_n = \operatorname{avi}(P_n) - an$. The following table gives values of c_n for small n:

n	1	2	3	4	5
c_n	$\frac{1}{2\sqrt{5}} \approx 0.2236$	$\frac{1}{\sqrt{5}} - \frac{1}{3} \approx 0.1139$	$\frac{3}{2\sqrt{5}} - \frac{1}{2} \approx 0.1708$	$\frac{2}{\sqrt{5}} - \frac{3}{4} \approx 0.1444$	$\frac{\sqrt{5}}{2} - \frac{25}{26} \approx 0.1565$

Table 4.1: Values of $c_1, c_2, \ldots, c_5$ for independent sets.

Before we prove our result, we require one more lemma:

Lemma 4.1.8. *For every tree T and every vertex v of T, we have*

$$\frac{1}{2} \leq \frac{\mathrm{I}(T-v)}{\mathrm{I}(T)} < 1.$$

Proof. Note first that $\mathrm{I}(T) = \mathrm{I}(T-v) + \mathrm{I}(T - N[v])$. Since $T - N[v]$ is a subgraph of $T - v$, we have $\mathrm{I}(T - N[v]) \leq \mathrm{I}(T-v)$, hence $2\mathrm{I}(T-v) \geq \mathrm{I}(T)$, which proves the first inequality. The second inequality simply follows from the fact that $T - v$ is a proper subgraph of T. ∎

Theorem 4.1.9. *For every tree T of order n that is not a path, we have the inequality* $\operatorname{avi}(T) \geq an + b$*, where* $b = (79\sqrt{5} - 165)/70 \approx 0.16641957$*. Consequently, the path minimises the value of* $\operatorname{avi}(T)$ *among all trees of order n.*

Proof. We prove the inequality by induction on n. For $n \leq 3$, there is nothing to prove since the only trees with three or fewer vertices are paths. Thus assume now that $n \geq 4$, and consider a vertex v of the tree T whose degree is at least 3 (which must exist if T is not a path). Denote the neighbours of v by $v_1, v_2, \ldots, v_k$ and the components of $T - v$ by $T_1, T_2, \ldots, T_k$ (in such a way that v_j is contained in T_j). We have

$$\begin{aligned}
\operatorname{avi}(T) &= \frac{\mathrm{T}(T)}{\mathrm{I}(T)} = \frac{\mathrm{T}(T-v) + (\mathrm{I}(T-N[v]) + \mathrm{T}(T-N[v]))}{\mathrm{I}(T)} \\
&= \frac{\mathrm{I}(T-v)}{\mathrm{I}(T)} \cdot \frac{\mathrm{T}(T-v)}{\mathrm{I}(T-v)} + \frac{\mathrm{I}(T-N[v])}{\mathrm{I}(T)} \cdot \Big(1 + \frac{\mathrm{T}(T-N[v])}{\mathrm{I}(T-N[v])}\Big) \\
&= \frac{\mathrm{I}(T-v)}{\mathrm{I}(T)} \operatorname{avi}(T-v) + \frac{\mathrm{I}(T) - \mathrm{I}(T-v)}{\mathrm{I}(T)} (1 + \operatorname{avi}(T-N[v])) \\
&= \frac{\mathrm{I}(T-v)}{\mathrm{I}(T)} \sum_{j=1}^{k} \operatorname{avi}(T_j) + \Big(1 - \frac{\mathrm{I}(T-v)}{\mathrm{I}(T)}\Big)\Big(1 + \sum_{j=1}^{k} \operatorname{avi}(T_j - v_j)\Big).
\end{aligned}$$

Assume first that $k \geq 5$, and let $T' = T - T_k$ be the tree obtained by removing T_k from T. Repeating the calculation, we also have

$$\operatorname{avi}(T') = \frac{\mathrm{I}(T'-v)}{\mathrm{I}(T')} \sum_{j=1}^{k-1} \operatorname{avi}(T_j) + \Big(1 - \frac{\mathrm{I}(T'-v)}{\mathrm{I}(T')}\Big)\Big(1 + \sum_{j=1}^{k-1} \operatorname{avi}(T_j - v_j)\Big).$$

For simplicity, let us introduce the notations $\rho = \frac{\mathrm{I}(T-v)}{\mathrm{I}(T)}$ and $\rho' = \frac{\mathrm{I}(T'-v)}{\mathrm{I}(T')}$. Note that

$$\rho = \frac{\mathrm{I}(T-v)}{\mathrm{I}(T)} = \frac{\prod_{j=1}^{k} \mathrm{I}(T_j)}{\prod_{j=1}^{k} \mathrm{I}(T_j) + \prod_{j=1}^{k} \mathrm{I}(T_j - v_j)} = \frac{1}{1 + \prod_{j=1}^{k} \frac{\mathrm{I}(T_j - v_j)}{\mathrm{I}(T_j)}} \tag{4.1.5}$$

and likewise

$$\rho' = \frac{1}{1 + \prod_{j=1}^{k-1} \frac{\mathrm{I}(T_j - v_j)}{\mathrm{I}(T_j)}},$$

so that Lemma 4.1.8 implies $\rho > \rho'$.

Now we write

$$\begin{aligned}
\operatorname{avi}(T) &= \rho \sum_{j=1}^{k} \operatorname{avi}(T_j) + (1-\rho)\Big(1 + \sum_{j=1}^{k} \operatorname{avi}(T_j - v_j)\Big) \\
&= \rho \operatorname{avi}(T_k) + (1-\rho) \operatorname{avi}(T_k - v_k) + \rho \sum_{j=1}^{k-1} \operatorname{avi}(T_j) \\
&\quad + (1-\rho)\Big(1 + \sum_{j=1}^{k-1} \operatorname{avi}(T_j - v_j).\Big)
\end{aligned}$$

$$\begin{aligned}\operatorname{avi}(T) &= \rho \operatorname{avi}(T_k) + (1-\rho)\operatorname{avi}(T_k - v_k) \\ &\quad + \frac{1-\rho}{1-\rho'}\Big(\rho' \sum_{j=1}^{k-1} \operatorname{avi}(T_j) + (1-\rho')\Big(1 + \sum_{j=1}^{k-1} \operatorname{avi}(T_j - v_j)\Big)\Big) \\ &\quad + \frac{\rho-\rho'}{1-\rho'} \sum_{j=1}^{k-1} \operatorname{avi}(T_j).\end{aligned}$$

By Lemma 4.1.7 and the induction hypothesis, we have $\operatorname{avi}(T_j) \geq a|T_j| + \frac{1}{\sqrt{5}} - \frac{1}{3}$ for all j. It follows that

$$\begin{aligned}\sum_{j=1}^{k-1} \operatorname{avi}(T_j) &\geq \sum_{j=1}^{k-1}\Big(a|T_j| + \frac{1}{\sqrt{5}} - \frac{1}{3}\Big) = a(|T'|-1) + (k-1)\Big(\frac{1}{\sqrt{5}} - \frac{1}{3}\Big) \\ &\geq a|T'| + 4\Big(\frac{1}{\sqrt{5}} - \frac{1}{3}\Big) - a > a|T'| + b.\end{aligned}$$

Moreover, the induction hypothesis gives us $\operatorname{avi}(T') \geq a|T'| + b$. Finally,

- If $|T_k| \geq 4$, then by the induction hypothesis and Lemma 4.1.7, we have

$$\begin{aligned}&\rho \operatorname{avi}(T_k) + (1-\rho)\operatorname{avi}(T_k - v_k) \\ &\geq \rho\Big(a|T_k| + \frac{2}{\sqrt{5}} - \frac{3}{4}\Big) + (1-\rho)\Big(a(|T_k|-1) + \frac{2}{\sqrt{5}} - \frac{3}{4}\Big) \\ &= a|T_k| + \frac{2}{\sqrt{5}} - \frac{3}{4} - (1-\rho)a \geq a|T_k| + \frac{2}{\sqrt{5}} - \frac{3}{4} - \frac{a}{2} > a|T_k|.\end{aligned}$$

- If $|T_k| = 3$, then $\rho \operatorname{avi}(T_k) + (1-\rho)\operatorname{avi}(T_k - v_k) \geq \rho + (1-\rho)\cdot\frac{2}{3} = \frac{2+\rho}{3} \geq \frac{5}{6} > 3a$ (by Lemma 4.1.8).

- If $|T_k| = 2$, then $\rho \operatorname{avi}(T_k) + (1-\rho)\operatorname{avi}(T_k - v_k) = \rho\cdot\frac{2}{3} + (1-\rho)\cdot\frac{1}{2} = \frac{3+\rho}{6} \geq \frac{7}{12} > 2a$ (by Lemma 4.1.8).

- If $|T_k| = 1$, then $\rho \operatorname{avi}(T_k) + (1-\rho)\operatorname{avi}(T_k - v_k) = \rho\cdot\frac{1}{2} + (1-\rho)\cdot 0 = \frac{\rho}{2}$, and since $\frac{\mathrm{I}(T_k - v_k)}{\mathrm{I}(T_k)} = \frac{1}{2}$ in this case, we have $\rho \geq \frac{2}{3}$ by (4.1.5). Thus $\rho \operatorname{avi}(T_k) + (1-\rho)\operatorname{avi}(T_k - v_k) \geq \frac{1}{3} > a$.

In conclusion, $\rho \operatorname{avi}(T_k) + (1-\rho)\operatorname{avi}(T_k - v_k) > a|T_k|$. Combining all inequalities, we obtain

$$\begin{aligned}\operatorname{avi}(T) &> a|T_k| + \frac{1-\rho}{1-\rho'}(a|T'| + b) + \frac{\rho-\rho'}{1-\rho'}(a|T'| + b) \\ &= a(|T'| + |T_k|) + b = a|T| + b.\end{aligned}$$

This completes the case that $k \geq 5$, so we are left with the cases $k = 3$ and $k = 4$. We return to the representation

$$\operatorname{avi}(T) = \rho \sum_{j=1}^{k} \operatorname{avi}(T_j) + (1-\rho)\Big(1 + \sum_{j=1}^{k} \operatorname{avi}(T_j - v_j)\Big). \tag{4.1.6}$$

Now we distinguish different cases depending on how many of the branches T_j have one, two or three vertices respectively. If T_j has three vertices, we also distinguish whether v_j is the centre vertex or a leaf of T_j. This gives us a total of 35 cases for $k = 3$ and 70 cases for $k = 4$, corresponding to the solutions of

$$x_1 + x_2 + x_3 + x_4 + x_5 = k.$$

Here, x_1 and x_2 stand for the number of T_j's with one and two vertices respectively, x_3 and x_4 the number of T_j's with three vertices and v_j the centre (x_3) or a leaf (x_4) respectively, and x_5 is the number of T_j's with four or more vertices. In each of the cases, we use the following explicit values and estimates:

$$\operatorname{avi}(T_j) \begin{cases} = \frac{1}{2} & |T_j| = 1, \\ = \frac{2}{3} & |T_j| = 2, \\ = 1 & |T_j| = 3, \\ \geq a|T_j| + \frac{2}{\sqrt{5}} - \frac{3}{4} & \text{otherwise}, \end{cases}$$

$$\operatorname{avi}(T_j - v_j) \begin{cases} = 0 & |T_j| = 1, \\ = \frac{1}{2} & |T_j| = 2, \\ = \frac{2}{3} & |T_j| = 3 \text{ and } v_j \text{ is a leaf of } T_j, \\ = 1 & |T_j| = 3 \text{ and } v_j \text{ is the centre of } T_j, \\ \geq a(|T_j| - 1) + \frac{2}{\sqrt{5}} - \frac{3}{4} & \text{otherwise}, \end{cases}$$

$$\frac{\mathrm{I}(T_j - v_j)}{\mathrm{I}(T_j)} \begin{cases} = \frac{1}{2} & |T_j| = 1, \\ = \frac{2}{3} & |T_j| = 2, \\ = \frac{3}{5} & |T_j| = 3 \text{ and } v_j \text{ is a leaf of } T_j, \\ = \frac{4}{5} & |T_j| = 3 \text{ and } v_j \text{ is the centre of } T_j, \\ \in [\frac{1}{2}, 1] & \text{otherwise}. \end{cases}$$

We plug these estimates into (4.1.6) and also use the identity (4.1.5) again. Since the expression (4.1.6) is linear in ρ, its minimum is either attained for the largest or smallest possible value of ρ. This gives us a lower bound for $\operatorname{avi}(T)$ in each of the aforementioned 105 cases, which can all be checked easily with a computer. As an example, let us consider the case that gives us the worst estimate: it is obtained for $x_1 = x_3 = x_4 = 0$, $x_2 = 1$ and $x_5 = 2$. Let T_1 and T_2 both have more than three vertices, so that the third branch T_3 consists of only two vertices. We have

$$\operatorname{avi}(T_1) \geq a|T_1| + \frac{2}{\sqrt{5}} - \frac{3}{4},\ \operatorname{avi}(T_2) \geq a|T_2| + \frac{2}{\sqrt{5}} - \frac{3}{4},\ \operatorname{avi}(T_3) = \frac{2}{3}$$

and

$$\begin{aligned}
\operatorname{avi}(T_1 - v_1) &\geq a|T_1| - a + \frac{2}{\sqrt{5}} - \frac{3}{4}, \\
\operatorname{avi}(T_2 - v_2) &\geq a|T_2| - a + \frac{2}{\sqrt{5}} - \frac{3}{4}, \\
\operatorname{avi}(T_3 - v_3) &= \frac{1}{2}
\end{aligned}$$

as well as

$$\rho = \frac{1}{1 + \frac{2}{3}\frac{\mathrm{I}(T_1 - v_1)\,\mathrm{I}(T_2 - v_2)}{\mathrm{I}(T_1)\,\mathrm{I}(T_2)}} \in \left[\frac{3}{5}, \frac{6}{7}\right].$$

Thus

$$\begin{aligned}
\operatorname{avi}(T_1) + \operatorname{avi}(T_2) + \operatorname{avi}(T_3) &\geq a(|T_1| + |T_2|) + 2\Big(\frac{2}{\sqrt{5}} - \frac{3}{4}\Big) + \frac{2}{3} \\
&= a|T| + \frac{4}{\sqrt{5}} - \frac{5}{6} - 3a \\
&= a|T| + \frac{11}{2\sqrt{5}} - \frac{7}{3}
\end{aligned}$$

and likewise

$$\begin{aligned}
&\operatorname{avi}(T_1 - v_1) + \operatorname{avi}(T_2 - v_2) + \operatorname{avi}(T_3 - v_3) \\
&\geq a(|T_1| + |T_2|) + 2\Big(\frac{2}{\sqrt{5}} - \frac{3}{4} - a\Big) + \frac{1}{2} \\
&= a|T| + \frac{4}{\sqrt{5}} - 1 - 5a \\
&= a|T| + \frac{13}{2\sqrt{5}} - \frac{7}{2}.
\end{aligned}$$

Putting everything together, we obtain

$$\begin{aligned}\operatorname{avi}(T) &\geq \rho\Big(a|T| + \frac{11}{2\sqrt{5}} - \frac{7}{3}\Big) + (1-\rho)\Big(1 + a|T| + \frac{13}{2\sqrt{5}} - \frac{7}{2}\Big)\\ &= a|T| + \frac{13}{2\sqrt{5}} - \frac{5}{2} + \rho\Big(\frac{1}{6} - \frac{1}{\sqrt{5}}\Big) \geq a|T| + \frac{13}{2\sqrt{5}} - \frac{5}{2} + \frac{6}{7}\Big(\frac{1}{6} - \frac{1}{\sqrt{5}}\Big)\\ &= a|T| + b.\end{aligned}$$

The other cases are treated in the same fashion and give lower bounds with larger constant terms. To complete the proof of the theorem, it only remains to prove an upper bound on $\operatorname{avi}(P_n)$. However, we already know from Lemma 4.1.7 that

$$\begin{aligned}\operatorname{avi}(P_n) &= an + \frac{3-\sqrt{5}}{5} - \frac{n+2}{\sqrt{5}((-\phi^2)^{n+2}-1)}\\ &\leq an + \frac{3-\sqrt{5}}{5} - \frac{7}{\sqrt{5}((-\phi^2)^7-1)} = an + \frac{\sqrt{5}}{2} - \frac{25}{26}\end{aligned}$$

for $n > 3$ and $\frac{\sqrt{5}}{2} - \frac{25}{26} \approx 0.15649553 < b$. Therefore, $\operatorname{avi}(P_n) < an + b \leq \operatorname{avi}(T)$ for every tree T with n vertices other than P_n. This completes the proof. ■

4.2 The weighted average size of independent sets in a graph

It is common in statistical physics to consider the hard-core distribution on the independent sets I of a graph G. That is, the study of a random independent set I with probability proportional to $\alpha^{|I|}$. In [12, 13], the authors use this model to prove bounds on the expected size of an independent set drawn from the hard-core model on G at fugacity α. This expected size coincides with the weighted average size that we consider. In our work, we characterize extremal graphs for the weighted average size of independent sets.

4.2.1 General considerations

Denote by $\mathrm{i}(G, k)$ the number of independent vertex subsets of size k in G. Now, let us consider a random independent set with probability proportional to α^k, where k is the size of the set and α is a positive number. We define the weighted total number of independent subsets of G, the weighted total size of independent subsets of G and the weighted average size of independent vertex subsets in G:

$$\begin{aligned} \mathrm{I}(G,\alpha) &= \sum_{k\geq 0} \mathrm{i}(G,k)\alpha^k, \\ \mathrm{T}(G,\alpha) &= \sum_{k\geq 0} k\,\mathrm{i}(G,k)\alpha^k, \\ \mathrm{avi}^{\alpha}(G) &= \frac{\mathrm{T}(G,\alpha)}{\mathrm{I}(G,\alpha)}. \end{aligned}$$

For ease of notation, we will use $\mathrm{I}^{\alpha}(G)$ instead of $\mathrm{I}(G,\alpha)$, as well as $\mathrm{T}^{\alpha}(G)$ for $\mathrm{T}(G,\alpha)$. Let us first compute $\mathrm{I}^{\alpha}, \mathrm{T}^{\alpha}, \mathrm{avi}^{\alpha}$ for the n-vertex edgeless graph E_n:

$$\begin{aligned} \mathrm{I}^{\alpha}(E_n) &= \sum_{k=0}^{n} \binom{n}{k}\alpha^k = (1+\alpha)^n \\ \mathrm{T}^{\alpha}(E_n) &= \sum_{k=0}^{n} \binom{n}{k} k\alpha^k = \alpha n(1+\alpha)^{n-1} \\ \mathrm{avi}^{\alpha}(E_n) &= \frac{\alpha n}{1+\alpha}. \end{aligned}$$

For the star S_n we have:

$$\begin{aligned} \mathrm{I}^{\alpha}(S_n) &= \alpha + \sum_{k=0}^{n-1} \binom{n-1}{k}\alpha^k = \alpha + (1+\alpha)^{n-1} \\ \mathrm{T}^{\alpha}(S_n) &= \alpha + \sum_{k=0}^{n} \binom{n-1}{k} k\alpha^k = \alpha + \alpha(n-1)(1+\alpha)^{n-2} \\ \mathrm{avi}^{\alpha}(S_n) &= \frac{\alpha + \alpha(n-1)(1+\alpha)^{n-2}}{\alpha + (1+\alpha)^{n-1}}. \end{aligned}$$

If v is a vertex of G and $N[v]$ its closed neighbourhood, then

$$\mathrm{T}^{\alpha}(G) = \mathrm{T}^{\alpha}(G-v) + \alpha\,\mathrm{T}^{\alpha}(G-N[v]) + \alpha\,\mathrm{I}^{\alpha}(G-N[v]), \tag{4.2.1}$$

which is obtained by summing up the cardinality of independent sets not containing v first and then that of those which contain v. With the well-known relation

$$\mathrm{I}^{\alpha}(G) = \mathrm{I}^{\alpha}(G-v) + \alpha\,\mathrm{I}^{\alpha}(G-N[v]),$$

(4.2.1) implies

$$\begin{aligned}\mathrm{avi}^{\alpha}(G) &= \frac{\mathrm{T}^{\alpha}(G-v)+\alpha\,\mathrm{T}^{\alpha}(G-N[v])+\alpha\,\mathrm{I}^{\alpha}(G-N[v])}{\mathrm{I}^{\alpha}(G-v)+\alpha\,\mathrm{I}^{\alpha}(G-N[v])}\\ &= \frac{\mathrm{avi}^{\alpha}(G-v)\,\mathrm{I}^{\alpha}(G-v)+\alpha(\mathrm{avi}^{\alpha}(G-N[v])+1)\,\mathrm{I}^{\alpha}(G-N[v])}{\mathrm{I}^{\alpha}(G-v)+\alpha\,\mathrm{I}^{\alpha}(G-N[v])}\end{aligned}$$

Theorem 4.2.1. *For any n-vertex graph G which is not the complete graph K_n,* $\mathrm{avi}^{\alpha}(K_n) < \mathrm{avi}^{\alpha}(G)$.

Proof. Since the only independent sets in K_n are the empty set and the n independent subsets of size 1, then the weighted average size of independent subsets in K_n is:

$$\mathrm{avi}^{\alpha}(K_n) = \frac{\alpha n}{1+\alpha n}.$$

For any other n-vertex graph, we have

$$\mathrm{avi}^{\alpha}(G) = \frac{\alpha n + \sum_{k\geq 2} k\,\mathrm{i}(G,k)\alpha^k}{1+\alpha n+\sum_{k\geq 2}\mathrm{i}(G,k)\alpha^k},$$

where $\sum_{k\geq 2} k\,\mathrm{i}(k,G)\alpha^k > \sum_{k\geq 2}\mathrm{i}(k,G)\alpha^k > 0$. Thus, we obtain:

$$\begin{aligned}&\mathrm{avi}^{\alpha}(G)-\mathrm{avi}^{\alpha}(K_n)\\ &= \frac{\alpha n + \sum_{k\geq 2} k\,\mathrm{i}(k,G)\alpha^k}{1+\alpha n+\sum_{k\geq 2}\mathrm{i}(k,G)\alpha^k} - \frac{\alpha n}{1+\alpha n}\\ &= \frac{(1+\alpha n)\left(\sum_{k\geq 2} k\,\mathrm{i}(k,G)\alpha^k\right)-\alpha n\left(\sum_{k\geq 2}\mathrm{i}(k,G)\alpha^k\right)}{\left(1+\alpha n+\sum_{k\geq 2}\mathrm{i}(k,G)\alpha^k\right)(1+\alpha n)}\\ &= \frac{\sum_{k\geq 2} k\,\mathrm{i}(k,G)\alpha^k+\alpha n\left(\sum_{k\geq 2} k\,\mathrm{i}(k,G)\alpha^k-\sum_{k\geq 2}\mathrm{i}(k,G)\alpha^k\right)}{\left(1+\alpha n+\sum_{k\geq 2}\mathrm{i}(k,G)\alpha^k\right)(1+\alpha n)}\\ &> 0.\end{aligned}$$

∎

Theorem 4.2.2. *For any n-vertex graph G which is not the edgeless graph E_n,*

$$\mathrm{avi}^{\alpha}(E_n) > \mathrm{avi}^{\alpha}(G).$$

Proof. Let us prove it by induction. For $n = 1$, the only possible graph is E_n, therefore the inequality is true.

Now, assume that the inequality is true for any $n \leq k$, for some $k \geq 1$. Let G be a $(k+1)$-vertex graph which is not edgeless, and $n = k+1$. Let $v \in V(G)$ be a vertex such that $\deg(v) \geq 1$. We have

$$\operatorname{avi}^{\alpha}(G) = \frac{\operatorname{avi}^{\alpha}(G-v)\,\mathrm{I}^{\alpha}(G-v) + \alpha(\operatorname{avi}^{\alpha}(G-N[v])+1)\,\mathrm{I}^{\alpha}(G-N[v])}{\mathrm{I}^{\alpha}(G-v)+\alpha\,\mathrm{I}^{\alpha}(G-N[v])}.$$

Using the induction hypothesis, we obtain

$$\begin{aligned}
\operatorname{avi}^{\alpha}(G) &\leq \frac{\frac{\alpha(n-1)}{1+\alpha}\,\mathrm{I}^{\alpha}(G-v) + \alpha(\frac{\alpha(n-2)}{1+\alpha}+1)(\mathrm{I}^{\alpha}(G-N[v]))}{\mathrm{I}^{\alpha}(G-v)+\alpha\,\mathrm{I}^{\alpha}(G-N[v])} \\
&= \frac{\alpha(n-1)}{1+\alpha} + \frac{\frac{1}{1+\alpha}\alpha\,\mathrm{I}^{\alpha}(G-N[v])}{\mathrm{I}^{\alpha}(G-v)+\alpha\,\mathrm{I}^{\alpha}(G-N[v])} \\
&< \frac{\alpha(n-1)}{1+\alpha} + \frac{1}{1+\alpha} = \frac{\alpha n}{1+\alpha} = \operatorname{avi}^{\alpha}(E_n).
\end{aligned}$$

■

4.2.2 The case of trees

Theorem 4.2.3. *For any n-vertex tree $T \neq S_n$, $\operatorname{avi}^{\alpha}(S_n) > \operatorname{avi}^{\alpha}(T)$.*

Proof. In the cases where $n = 1, 2, 3$, we must have $G = S_n$, and thus the claim holds.

Assume the inequality is true for all $n \leq k$, for some $k \geq 3$. Now suppose that $G \neq S_n$ is a tree with $n = k+1$ vertices. Let $v \in V(T)$ be a leaf of T. Then $T - v$ is again a tree, we have $\mathrm{I}^{\alpha}(T-v) < \mathrm{I}^{\alpha}(S_{n-1}) = \alpha + (1+\alpha)^{n-2}$ and $\mathrm{I}^{\alpha}(T-v) - \mathrm{I}^{\alpha}(T-N[v]) > \alpha$, so

$$\begin{aligned}
\frac{\mathrm{I}^{\alpha}(T-N[v])}{\mathrm{I}^{\alpha}(T-v)} &= 1 - \frac{\mathrm{I}^{\alpha}(T-v)-\mathrm{I}^{\alpha}(T-N[v])}{\mathrm{I}^{\alpha}(T-v)} \\
&< 1 - \frac{\alpha}{\mathrm{I}^{\alpha}(T-v)} \leq 1 - \frac{\alpha}{\alpha+(1+\alpha)^{n-2}},
\end{aligned}$$

and thus

$$\frac{\mathrm{I}^{\alpha}(T-v)}{\mathrm{I}^{\alpha}(T-N[v])} \geq \frac{\alpha+(1+\alpha)^{n-2}}{(1+\alpha)^{n-2}}. \tag{4.2.2}$$

Using the induction hypothesis and Theorem 4.2.2, we obtain:

$$\begin{aligned}\operatorname{avi}^{\alpha}(G) &= \frac{\operatorname{avi}^{\alpha}(T-v)\,\mathrm{I}^{\alpha}(T-v) + \alpha(\operatorname{avi}^{\alpha}(T-N[v])+1)\,\mathrm{I}^{\alpha}(T-N[v])}{\mathrm{I}^{\alpha}(T-v)+\alpha\,\mathrm{I}^{\alpha}(T-N[v])} \\ &\le \frac{\operatorname{avi}^{\alpha}(S_{n-1})\,\mathrm{I}^{\alpha}(T-v)/\,\mathrm{I}^{\alpha}(T-N[v]) + \frac{\alpha^2(n-2)}{1+\alpha}+\alpha}{\mathrm{I}^{\alpha}(T-v)/\,\mathrm{I}^{\alpha}(T-N[v])+\alpha}.\end{aligned}$$

Since $\operatorname{avi}^{\alpha}(S_{n-1}) < \frac{\alpha(n-2)}{1+\alpha}+1$, $\frac{\operatorname{avi}^{\alpha}(S_{n-1})x+\frac{\alpha^2(n-2)}{1+\alpha}+\alpha}{x+\alpha}$ is decreasing for $x \ge 0$, and using Equation (4.2.2), we get

$$\begin{aligned}\operatorname{avi}^{\alpha}(T) &< \frac{\operatorname{avi}^{\alpha}(S_{n-1})(\alpha+(1+\alpha)^{n-2})/(1+\alpha)^{n-2} + \frac{\alpha^2(n-2)}{1+\alpha}+\alpha}{(\alpha+(1+\alpha)^{n-2})/(1+\alpha)^{n-2}+\alpha} \\ &= \frac{\mathrm{T}^{\alpha}(S_{n-1}) + \alpha^2(n-2)(1+\alpha)^{n-3}+\alpha(1+\alpha)^{n-2}}{\alpha+(1+\alpha)^{n-1}} \\ &= \frac{\alpha+\alpha(n-2)(1+\alpha)^{n-3}+\alpha^2(n-2)(1+\alpha)^{n-3}+\alpha(1+\alpha)^{n-2}}{\alpha+(1+\alpha)^{n-1}} \\ &= \operatorname{avi}^{\alpha}(S_n).\end{aligned}$$

■

For the problem of minimizing the weighted average size of independent sets in a tree, we have to consider different cases depending on α. So first, let us consider $\alpha \in [0,1]$. As for the average size of independent sets, let us find an explicit formula for the weighted average size of independent sets in a path.

Lemma 4.2.4. *The weighted average size of independent sets of the n-vertex path P_n is*

$$\begin{aligned}\operatorname{avi}^{\alpha}(P_n) = \frac{1+4\alpha-\sqrt{1+4\alpha}}{2(1+4\alpha)}n + \frac{1+2\alpha-\sqrt{1+4\alpha}}{1+4\alpha} \\ - \frac{(n+2)\alpha^{n+2}}{\sqrt{1+4\alpha}((-\phi_{\alpha}^2)^{n+2}-\alpha^{n+2})},\end{aligned} \tag{4.2.3}$$

where $\phi_\alpha = \frac{\sqrt{1+4\alpha}+1}{2}$. In particular,

(a) $\lim_{n\to\infty} \operatorname{avi}^{\alpha}(P_n) - \frac{1+4\alpha-\sqrt{1+4\alpha}}{2(1+4\alpha)}n = \frac{1+2\alpha-\sqrt{1+4\alpha}}{1+4\alpha}$,

(b) $\operatorname{avi}^{\alpha}(P_n) \ge \frac{1+4\alpha-\sqrt{1+4\alpha}}{2(1+4\alpha)}n + \frac{1}{\sqrt{1+4\alpha}} - \frac{1}{1+2\alpha}$, *with equality only for $n = 2$. For all positive integers $n \ne 2$, we even have* $\operatorname{avi}^{\alpha}(P_n) \ge \frac{1+4\alpha-\sqrt{1+4\alpha}}{2(1+4\alpha)}n + \frac{2}{\sqrt{1+4\alpha}} - \frac{2(1+2\alpha)}{1+4\alpha+3\alpha^2}$.

Proof. The weighted number of independent sets of P_n follows the following recursion: $\mathrm{I}^\alpha(P_n) = \mathrm{I}^\alpha(P_{n-1}) + \alpha\,\mathrm{I}^\alpha(P_{n-2})$. We solve this recursion and obtain that

$$\mathrm{I}^\alpha(P_n) = \frac{1}{\sqrt{1+4\alpha}}\big(\phi_\alpha^{n+2} - (1-\phi_\alpha)^{n+2}\big).$$

The weighted total number of vertices $\mathrm{T}^\alpha(P_n)$ in all independent sets of P_n is determined by the recursion

$$\mathrm{T}^\alpha(P_n) = \mathrm{T}^\alpha(P_{n-1}) + \alpha\,\mathrm{T}^\alpha(P_{n-2}) + \alpha\,\mathrm{I}^\alpha(P_{n-2})$$

and the initial values $\mathrm{T}^\alpha(P_0) = 0$, $\mathrm{T}^\alpha(P_1) = \alpha$, $\mathrm{T}^\alpha(P_2) = 2\alpha$ and $\mathrm{T}^\alpha(P_3) = 3\alpha + 2\alpha^2$. We get:

$$\begin{aligned}&\mathrm{T}^\alpha(P_n)\\ &= \left(\frac{2\alpha^2\sqrt{1+4\alpha}}{(1+4\alpha)^2} + \frac{n\alpha\phi_\alpha}{1+4\alpha}\right)\phi_\alpha^n - \left(\frac{2\alpha^2\sqrt{1+4\alpha}}{(1+4\alpha)^2} + \frac{n\alpha(\phi_\alpha - 1)}{1+4\alpha}\right)(1-\phi_\alpha)^n.\end{aligned}$$

Using the fact that $\alpha = \phi_\alpha(\phi_\alpha - 1)$, we obtain the formula (4.2.3) for the quotient $\mathrm{avi}^\alpha(P_n) = \mathrm{T}^\alpha(P_n)/\,\mathrm{I}^\alpha(P_n)$, as well as the limit in (a).

Now we show that the absolute value of the error term is decreasing: for $n \geq 2$, we have

$$\begin{aligned}\left|\frac{\frac{(n+2)\alpha^{n+2}}{\sqrt{1+4\alpha}((-\phi_\alpha^2)^{n+2}-\alpha^{n+2})}}{\frac{(n+1)\alpha^{n+1}}{\sqrt{1+4\alpha}((-\phi_\alpha^2)^{n+1}-\alpha^{n+1})}}\right| &\leq \alpha\left(1+\frac{1}{n+1}\right)\cdot\frac{\phi_\alpha^{2(n+1)} + \alpha^{n+1}}{\phi_\alpha^{2(n+2)} - \alpha^{n+2}}\\ &= \alpha\cdot\phi_\alpha^{-2}\left(1+\frac{1}{n+1}\right)\cdot\frac{\alpha^{n+1}\phi_\alpha^{-2(n+1)}+1}{1-\alpha^{n+2}\phi_\alpha^{-2(n+2)}}\\ &\leq \phi_\alpha^{-2}\cdot\frac{4}{3}\cdot\alpha\cdot\frac{\phi_\alpha^{-6}+1}{1-\phi_\alpha^{-8}} = R(\alpha).\end{aligned}$$

The function $R(\alpha)$ is increasing in terms of $\alpha \in [0,1]$, thus $R(\alpha) \leq R(1) < 1$, therefore the difference

$$\left|\mathrm{avi}^\alpha(P_n) - \frac{1+4\alpha-\sqrt{1+4\alpha}}{2(1+4\alpha)}n - \frac{1+2\alpha-\sqrt{1+4\alpha}}{1+4\alpha}\right|$$

is decreasing in n. Moreover, note that the sign of $\frac{(n+2)\alpha^{n+2}}{\sqrt{1+4\alpha}((-\phi^2)^{n+2}-\alpha^{n+2})}$ alternates, so that $\mathrm{avi}^\alpha(P_n)$ is alternatingly greater and less than $\frac{1+4\alpha-\sqrt{1+4\alpha}}{2(1+4\alpha)}n + \frac{1+2\alpha-\sqrt{1+4\alpha}}{1+4\alpha}$. It follows that the minimum of the difference between $\mathrm{avi}^\alpha(P_n)$

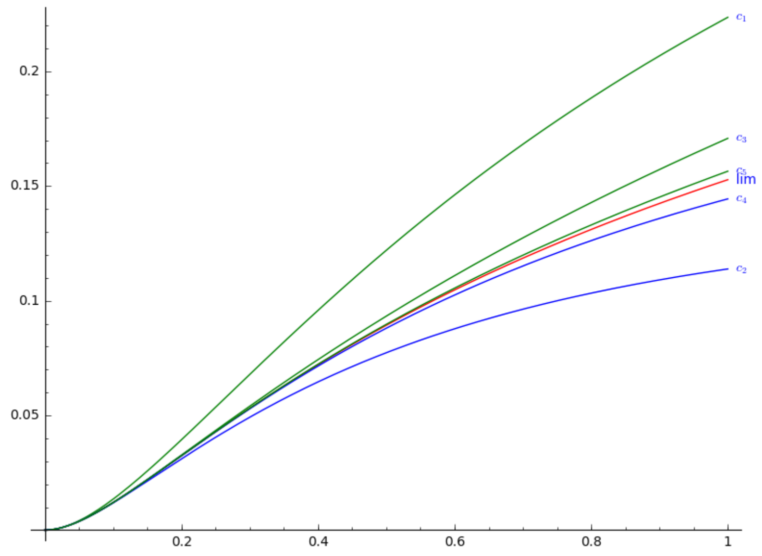


Figure 4.1: Values of $c_n(\alpha)$ for $n = 1, \ldots, 5$ and the limit $\frac{1+2\alpha-\sqrt{1+4\alpha}}{1+4\alpha}$.

and $\frac{1+4\alpha-\sqrt{1+4\alpha}}{2(1+4\alpha)}n$ is attained for $n = 2$. Among all $n \neq 2$, the minimum occurs when $n = 4$. The values of $\mathrm{avi}^{\alpha}(P_n)$ are easily calculated in both cases, and the two inequalities in (b) follow. ■

For ease of notation, we set $a = \frac{1+4\alpha-\sqrt{1+4\alpha}}{2(1+4\alpha)}$ and $c_n(\alpha) = \mathrm{avi}^{\alpha}(P_n) - an$. Let us give values of $c_n(\alpha)$ (also shown in Figure 4.1) for small n:

$$
\begin{aligned}
c_1(\alpha) &= \frac{\alpha-1}{2(\alpha+1)} + \frac{1}{2\sqrt{1+4\alpha}} \\
c_2(\alpha) &= -\frac{1}{2\alpha+1} + \frac{1}{\sqrt{1+4\alpha}} \\
c_3(\alpha) &= \frac{\alpha^2-3\alpha-3}{2(\alpha^2+3\alpha+1)} + \frac{3}{2\sqrt{1+4\alpha}} \\
c_4(\alpha) &= -\frac{2(2\alpha+1)}{3\alpha^2+4\alpha+1} + \frac{2}{\sqrt{1+4\alpha}} \\
c_5(\alpha) &= \frac{\alpha^3-6\alpha^2-15\alpha-5}{2(\alpha^3+6\alpha^2+5\alpha+1)} + \frac{5}{2\sqrt{1+4\alpha}}.
\end{aligned}
$$

Before proving our result, we require one more lemma:

Lemma 4.2.5. *For every tree T and every vertex v of T, we have*

$$\frac{1}{\alpha+1} \leq \frac{\mathrm{I}^{\alpha}(T-v)}{\mathrm{I}^{\alpha}(T)} < 1.$$

Proof. Note first that $\mathrm{I}^\alpha(T) = \mathrm{I}^\alpha(T-v) + \alpha\,\mathrm{I}^\alpha(T-N[v])$. Since $T-N[v]$ is a subgraph of $T-v$, we have $\mathrm{I}^\alpha(T-N[v]) \le \mathrm{I}^\alpha(T-v)$, hence $(1+\alpha)\,\mathrm{I}^\alpha(T-v) \ge \mathrm{I}^\alpha(T)$, which proves the first inequality. The second inequality simply follows from the fact that $T-v$ is a proper subgraph of T. ∎

Theorem 4.2.6. *For every $\alpha \in (0,1]$ and every tree T of order n that is not a path, we have the inequality $\mathrm{avi}^\alpha(T) \ge an + c_5(\alpha)$. Consequently, the path minimises the value of $\mathrm{avi}^\alpha(T)$ among all trees of order n.*

Proof. We prove the inequality by induction on n. For $n \le 3$, there is nothing to prove since the only trees with three or fewer vertices are paths. Thus assume now that $n \ge 4$, and consider a vertex v of the tree T whose degree is at least 3 (which must exist if T is not a path). Denote the neighbours of v by $v_1, v_2, \ldots, v_k$ and the components of $T-v$ by $T_1, T_2, \ldots, T_k$ (in such a way that v_j is contained in T_j). We have

$$\begin{aligned}
\mathrm{avi}^\alpha(T) &= \frac{\mathrm{T}^\alpha(T)}{\mathrm{I}^\alpha(T)} = \frac{\mathrm{T}^\alpha(T-v) + \alpha(\mathrm{I}^\alpha(T-N[v]) + \mathrm{T}^\alpha(T-N[v]))}{\mathrm{I}^\alpha(T)} \\
&= \frac{\mathrm{I}^\alpha(T-v)}{\mathrm{I}^\alpha(T)} \cdot \frac{\mathrm{T}^\alpha(T-v)}{\mathrm{I}^\alpha(T-v)} + \frac{\alpha\,\mathrm{I}^\alpha(T-N[v])}{\mathrm{I}^\alpha(T)} \cdot \left(1 + \frac{\mathrm{T}^\alpha(T-N[v]^\alpha)}{\mathrm{I}^\alpha(T-N[v])}\right) \\
&= \frac{\mathrm{I}^\alpha(T-v)}{\mathrm{I}^\alpha(T)}\,\mathrm{avi}^\alpha(T-v) + \frac{\mathrm{I}^\alpha(T) - \mathrm{I}^\alpha(T-v)}{\mathrm{I}^\alpha(T)}(1 + \mathrm{avi}^\alpha(T-N[v])) \\
&= \frac{\mathrm{I}^\alpha(T-v)}{\mathrm{I}^\alpha(T)} \sum_{j=1}^{k} \mathrm{avi}^\alpha(T_j) + \left(1 - \frac{\mathrm{I}^\alpha(T-v)}{\mathrm{I}^\alpha(T)}\right)\left(1 + \sum_{j=1}^{k} \mathrm{avi}^\alpha(T_j - v_j)\right).
\end{aligned}$$

Assume first that $k \ge 5$, and let $T' = T - T_k$ be the tree obtained by removing T_k from T. Repeating the calculation, we also have

$$\mathrm{avi}^\alpha(T') = \frac{\mathrm{I}^\alpha(T'-v)}{\mathrm{I}^\alpha(T')} \sum_{j=1}^{k-1} \mathrm{avi}^\alpha(T_j) + \left(1 - \frac{\mathrm{I}^\alpha(T'-v)}{\mathrm{I}^\alpha(T')}\right)\left(1 + \sum_{j=1}^{k-1} \mathrm{avi}^\alpha(T_j - v_j)\right).$$

For simplicity, let us introduce the notations $\rho_\alpha = \frac{\mathrm{I}^\alpha(T-v)}{\mathrm{I}^\alpha(T)}$ and $\rho'_\alpha = \frac{\mathrm{I}^\alpha(T'-v)}{\mathrm{I}^\alpha(T')}$. Note that

$$\rho_\alpha = \frac{\mathrm{I}^\alpha(T-v)}{\mathrm{I}^\alpha(T)} = \frac{\prod_{j=1}^{k} \mathrm{I}^\alpha(T_j)}{\prod_{j=1}^{k} \mathrm{I}^\alpha(T_j) + \alpha \prod_{j=1}^{k} \mathrm{I}^\alpha(T_j - v_j)} = \frac{1}{1 + \alpha \prod_{j=1}^{k} \frac{\mathrm{I}^\alpha(T_j - v_j)}{\mathrm{I}^\alpha(T_j)}} \tag{4.2.4}$$

and likewise

$$\rho'_\alpha = \frac{1}{1 + \alpha \prod_{j=1}^{k-1} \frac{\mathrm{I}^\alpha(T_j - v_j)}{\mathrm{I}^\alpha(T_j)}},$$

so that Lemma 4.2.5 implies $\rho_\alpha > \rho'_\alpha$. Now we write

$$\begin{aligned}
\operatorname{avi}^\alpha(T) &= \rho_\alpha \sum_{j=1}^{k} \operatorname{avi}^\alpha(T_j) + (1-\rho_\alpha)\Big(1 + \sum_{j=1}^{k} \operatorname{avi}^\alpha(T_j - v_j)\Big) \\
&= \rho_\alpha \operatorname{avi}^\alpha(T_k) + (1-\rho_\alpha)\operatorname{avi}^\alpha(T_k - v_k) + \rho_\alpha \sum_{j=1}^{k-1} \operatorname{avi}^\alpha(T_j) \\
&\quad + (1-\rho_\alpha)\Big(1 + \sum_{j=1}^{k-1} \operatorname{avi}^\alpha(T_j - v_j)\Big)
\end{aligned}$$

and thus

$$\begin{aligned}
\operatorname{avi}^\alpha(T) &= \rho_\alpha \operatorname{avi}^\alpha(T_k) + (1-\rho_\alpha)\operatorname{avi}^\alpha(T_k - v_k) \\
&\quad + \frac{1-\rho_\alpha}{1-\rho'_\alpha}\bigg(\rho'_\alpha \sum_{j=1}^{k-1} \operatorname{avi}^\alpha(T_j) + (1-\rho'_\alpha)\Big(1 + \sum_{j=1}^{k-1} \operatorname{avi}^\alpha(T_j - v_j)\Big)\bigg) \\
&\quad + \frac{\rho_\alpha - \rho'_\alpha}{1-\rho'_\alpha} \sum_{j=1}^{k-1} \operatorname{avi}^\alpha(T_j) \\
&= \rho_\alpha \operatorname{avi}^\alpha(T_k) + (1-\rho_\alpha)\operatorname{avi}^\alpha(T_k - v_k) + \frac{1-\rho_\alpha}{1-\rho'_\alpha}\operatorname{avi}^\alpha(T') \\
&\quad + \left(1 - \frac{1-\rho_\alpha}{1-\rho'_\alpha}\right) \sum_{j=1}^{k-1} \operatorname{avi}^\alpha(T_j). \qquad (4.2.5)
\end{aligned}$$

Let us consider the following cases:

- If $|T_k| \geq 4$, then by the induction hypothesis and Lemma 4.2.4, we have

$$\begin{aligned}
&\rho_\alpha \operatorname{avi}^\alpha(T_k) + (1-\rho_\alpha)\operatorname{avi}^\alpha(T_k - v_k) \\
&\geq \rho_\alpha\Big(a|T_k| + c_4(\alpha)\Big) + (1-\rho_\alpha)\Big(a(|T_k|-1) + c_4(\alpha)\Big) \\
&= a|T_k| + c_4(\alpha) - (1-\rho_\alpha)a \geq a|T_k| + c_4(\alpha) - \frac{a\alpha}{\alpha+1} > a|T_k|.
\end{aligned}$$

- If $|T_k| = 3$, then

$$\begin{aligned}
&\rho_\alpha \operatorname{avi}^\alpha(T_k) + (1-\rho_\alpha)\operatorname{avi}^\alpha(T_k - v_k) \\
&\geq \rho_\alpha \cdot \frac{2\alpha^2+3\alpha}{\alpha^2+3\alpha+1} + (1-\rho_\alpha)\cdot\frac{2\alpha}{2\alpha+1} \\
&= \frac{(2\alpha^3+2\alpha^2+\alpha)\rho_\alpha + 2\alpha^3+6\alpha^2+2\alpha}{2\alpha^3+7\alpha^2+5\alpha+1}.
\end{aligned}$$

By Lemma 4.2.5, $\rho_\alpha \geq \frac{1}{1+\alpha}$, hence

$$\begin{aligned}&\rho_\alpha \operatorname{avi}^\alpha(T_k) + (1-\rho_\alpha)\operatorname{avi}^\alpha(T_k - v_k)\\&\geq \frac{2\alpha^4 + 10\alpha^3 + 10\alpha^2 + 3\alpha}{2\alpha^4 + 9\alpha^3 + 12\alpha^2 + 6\alpha + 1} > 3a.\end{aligned}$$

- If $|T_k| = 2$, then

$$\begin{aligned}&\rho_\alpha \operatorname{avi}^\alpha(T_k) + (1-\rho_\alpha)\operatorname{avi}^\alpha(T_k - v_k)\\&= \rho_\alpha \cdot \frac{2\alpha}{2\alpha+1} + (1-\rho_\alpha)\cdot\frac{\alpha}{\alpha+1} = \frac{2\alpha^2 + \alpha + \rho_\alpha\alpha}{2\alpha^2 + 3\alpha + 1},\end{aligned}$$

So by Lemma 4.2.5 again, we have

$$\rho_\alpha \operatorname{avi}^\alpha(T_k) + (1-\rho_\alpha)\operatorname{avi}^\alpha(T_k - v_k) \geq \frac{2\alpha^3 + 3\alpha^2 + 2\alpha}{2\alpha^3 + 5\alpha^2 + 4\alpha + 1} > 2a.$$

- If $|T_k| = 1$, then

$$\rho_\alpha \operatorname{avi}^\alpha(T_k) + (1-\rho_\alpha)\operatorname{avi}^\alpha(T_k - v_k) = \rho_\alpha \cdot \frac{\alpha}{\alpha+1} + (1-\rho_\alpha)\cdot 0 = \frac{\rho_\alpha\alpha}{\alpha+1},$$

and since $\frac{\mathrm{I}^\alpha(T_k - v_k)}{\mathrm{I}^\alpha(T_k)} = \frac{1}{\alpha+1}$ in this case, we have $\rho_\alpha \geq \frac{\alpha+1}{2\alpha+1}$ by (4.2.4). Thus $\rho_\alpha \operatorname{avi}^\alpha(T_k) + (1-\rho_\alpha)\operatorname{avi}^\alpha(T_k - v_k) \geq \frac{\alpha}{2\alpha+1} > a$.

In summary, $\rho_\alpha \operatorname{avi}^\alpha(T_k) + (1-\rho_\alpha)\operatorname{avi}^\alpha(T_k - v_k) > a|T_k|$. Moreover, the induction hypothesis gives us $\operatorname{avi}^\alpha(T') \geq a|T'| + c_5(\alpha)$. If $\sum_{j=1}^{k-1}\operatorname{avi}^\alpha(T_j) \geq \operatorname{avi}^\alpha(T')$, then we are done. So we may assume that $\sum_{j=1}^{k-1}\operatorname{avi}^\alpha(T_j) < \operatorname{avi}^\alpha(T')$, so that $\frac{1-\rho_\alpha}{1-\rho'_\alpha}\operatorname{avi}^\alpha(T') + \left(1 - \frac{1-\rho_\alpha}{1-\rho'_\alpha}\right)\sum_{j=1}^{k-1}\operatorname{avi}^\alpha(T_j)$ is an increasing function of $\frac{1-\rho_\alpha}{1-\rho'_\alpha}$. Let us find a lower bound for $\frac{1-\rho_\alpha}{1-\rho'_\alpha}$. We have:

$$\begin{aligned}\frac{1-\rho_\alpha}{1-\rho'_\alpha} &= \frac{\alpha\prod_{j=1}^{k}\frac{\mathrm{I}^\alpha(T_j - v_j)}{\mathrm{I}^\alpha(T_j)}}{1 + \alpha\prod_{j=1}^{k}\frac{\mathrm{I}^\alpha(T_j - v_j)}{\mathrm{I}^\alpha(T_j)}} \cdot \frac{1 + \alpha\prod_{j=1}^{k-1}\frac{\mathrm{I}^\alpha(T_j - v_j)}{\mathrm{I}^\alpha(T_j)}}{\alpha\prod_{j=1}^{k-1}\frac{\mathrm{I}^\alpha(T_j - v_j)}{\mathrm{I}^\alpha(T_j)}}\\&\geq \frac{\mathrm{I}^\alpha(T_k - v_k)}{\mathrm{I}^\alpha(T_k)}.\end{aligned}$$

Therefore, from Equation (4.2.5), we obtain

$$\begin{aligned}\operatorname{avi}^\alpha(T) \geq{}& \rho_\alpha \operatorname{avi}^\alpha(T_k) + (1-\rho_\alpha)\operatorname{avi}^\alpha(T_k - v_k) + \frac{\mathrm{I}^\alpha(T_k - v_k)}{\mathrm{I}^\alpha(T_k)}\operatorname{avi}^\alpha(T')\\&+ \left(1 - \frac{\mathrm{I}^\alpha(T_k - v_k)}{\mathrm{I}^\alpha(T_k)}\right)\sum_{j=1}^{k-1}\operatorname{avi}^\alpha(T_j).\end{aligned}$$

By Lemma 4.2.4 and the induction hypothesis, we have $\mathrm{avi}^{\alpha}(T_j) \geq a|T_j| + c_2(\alpha)$ for all j. It follows that

$$\begin{aligned}\sum_{j=1}^{k-1} \mathrm{avi}^{\alpha}(T_j) &\geq \sum_{j=1}^{k-1} \Big(a|T_j| + c_2(\alpha) \Big) = a(|T'| - 1) + (k-1)c_2(\alpha) \\ &\geq a|T'| + 4c_2(\alpha) - a.\end{aligned}$$

Let us consider again the following cases:

- If $|T_k| \geq 4$, we have $\frac{\mathrm{I}^{\alpha}(T_k - v_k)}{\mathrm{I}^{\alpha}(T_k)} \geq \frac{1}{\alpha+1}$. Moreover, by the induction hypothesis and Lemma 4.2.4, we obtain

$$\begin{aligned}\mathrm{avi}^{\alpha}(T) \geq a|T_k| &+ c_4(\alpha) - \frac{a\alpha}{\alpha+1} \\ &+ \frac{1}{\alpha+1}(a|T'| + c_5(\alpha)) + \frac{\alpha}{\alpha+1}(a|T'| + 4c_2(\alpha) - a) \\ = a|T| &+ c_4(\alpha) - \frac{a\alpha}{\alpha+1} \\ &+ \frac{1}{\alpha+1}(c_5(\alpha) + \alpha(4c_2(\alpha) - a)) \geq a|T| + c_5(\alpha).\end{aligned}$$

- If $|T_k| = 3$, we have $\frac{\mathrm{I}^{\alpha}(T_k - v_k)}{\mathrm{I}^{\alpha}(T_k)} \geq \frac{2\alpha+1}{\alpha^2+3\alpha+1}$. Moreover, by the induction hypothesis and Lemma 4.2.4, we obtain

$$\begin{aligned}\mathrm{avi}^{\alpha}(T) &\geq a|T_k| + \frac{2\alpha^4 + 10\alpha^3 + 10\alpha^2 + 3\alpha}{2\alpha^4 + 9\alpha^3 + 12\alpha^2 + 6\alpha + 1} - 3a \\ &+ \frac{2\alpha+1}{\alpha^2+3\alpha+1}(a|T'| + c_5(\alpha)) + \frac{\alpha^2+\alpha}{\alpha^2+3\alpha+1}(a|T'| + 4c_2(\alpha) - a) \\ &= a|T| + \frac{2\alpha^4 + 10\alpha^3 + 10\alpha^2 + 3\alpha}{2\alpha^4 + 9\alpha^3 + 12\alpha^2 + 6\alpha + 1} - 3a \\ &+ \frac{1}{\alpha^2+3\alpha+1}((2\alpha+1)c_5(\alpha) + (\alpha^2+\alpha)(4c_2(\alpha) - a)) \\ &\geq a|T| + c_5(\alpha).\end{aligned}$$

- If $|T_k| = 2$, we have $\frac{\mathrm{I}^{\alpha}(T_k - v_k)}{\mathrm{I}^{\alpha}(T_k)} = \frac{\alpha+1}{2\alpha+1}$. Moreover, by the induction hypothesis and Lemma 4.2.4, we obtain

$$\begin{aligned}
\operatorname{avi}^{\alpha}(T) &\geq a|T_k| + \frac{2\alpha^3+3\alpha^2+2\alpha}{2\alpha^3+5\alpha^2+4\alpha+1} - 2a \\
&\quad + \frac{\alpha+1}{2\alpha+1}(a|T'| + c_5(\alpha)) + \frac{\alpha}{2\alpha+1}(a|T'| + 4c_2(\alpha) - a) \\
&= a|T| + \frac{2\alpha^3+3\alpha^2+2\alpha}{2\alpha^3+5\alpha^2+4\alpha+1} - 2a \\
&\quad + \frac{1}{2\alpha+1}((\alpha+1)c_5(\alpha) + \alpha(4c_2(\alpha) - a)) \geq a|T| + c_5(\alpha).
\end{aligned}$$

- If $|T_k| = 1$, we have $\frac{\mathrm{I}^{\alpha}(T_k - v_k)}{\mathrm{I}^{\alpha}(T_k)} = \frac{1}{\alpha+1}$. Moreover, by the induction hypothesis and Lemma 4.2.4, we obtain

$$\begin{aligned}
\operatorname{avi}^{\alpha}(T) &\geq a|T_k| + \frac{\alpha}{2\alpha+1} - a + \frac{1}{\alpha+1}(a|T'| + c_5(\alpha)) \\
&\quad + \frac{\alpha}{\alpha+1}(a|T'| + 4c_2(\alpha) - a) \\
&\geq a|T| + \frac{\alpha}{2\alpha+1} - a + \frac{1}{\alpha+1}(c_5(\alpha) + \alpha(4c_2(\alpha) - a)) \\
&\geq a|T| + c_5(\alpha).
\end{aligned}$$

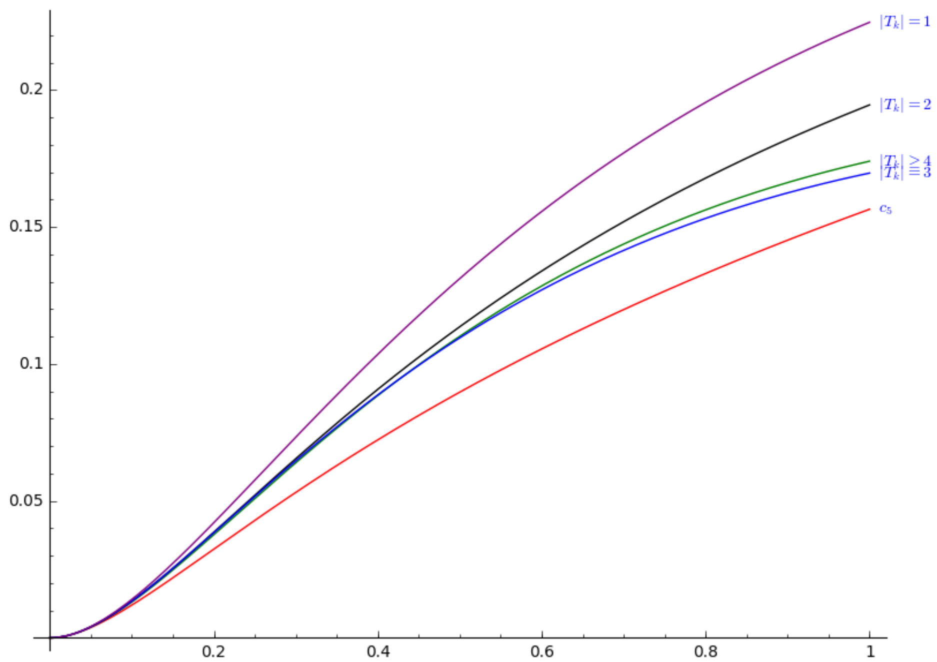


Figure 4.2: The four different cases in comparison to $c_5(\alpha)$.

This completes the case that $k \geq 5$, so we are left with the cases $k = 3$ and $k = 4$. We return to the representation

$$\operatorname{avi}^\alpha(T) = \rho_\alpha \sum_{j=1}^{k} \operatorname{avi}^\alpha(T_j) + (1-\rho_\alpha)\Big(1 + \sum_{j=1}^{k} \operatorname{avi}^\alpha(T_j - v_j)\Big) \tag{4.2.6}$$

Now we distinguish different cases depending on how many of the branches T_j have one, two or three vertices respectively. If T_j has three vertices, we also distinguish whether v_j is the centre vertex or a leaf of T_j. This gives us a total of 35 cases for $k = 3$ and 70 cases for $k = 4$, corresponding to the solutions of

$$x_1 + x_2 + x_3 + x_4 + x_5 = k.$$

Here, x_1 and x_2 stand for the number of T_j's with one and two vertices respectively, x_3 and x_4 the number of T_j's with three vertices and v_j the centre (x_3) or a leaf (x_4) respectively, and x_5 is the number of T_j's with four or more vertices. In each of the cases, we use the following explicit values and estimates:

$$\operatorname{avi}^\alpha(T_j) \begin{cases} = a|T_j| + c_1(\alpha) & |T_j| = 1, \\ = a|T_j| + c_2(\alpha) & |T_j| = 2, \\ = a|T_j| + c_3(\alpha) & |T_j| = 3, \\ \geq a|T_j| + c_4(\alpha) & \text{otherwise}, \end{cases}$$

$$\operatorname{avi}^\alpha(T_j - v_j) \begin{cases} = a|T_j| - a & |T_j| = 1, \\ = a|T_j| + c_1(\alpha) - a & |T_j| = 2, \\ = a|T_j| + c_2(\alpha) - a & |T_j| = 3 \text{ and } v_j \text{ is a leaf of } T_j, \\ = a|T_j| + 2c_1(\alpha) - a & |T_j| = 3 \text{ and } v_j \text{ is the centre of } T_j, \\ \geq a|T_j| + c_4(\alpha) - a & \text{otherwise}, \end{cases}$$

$$\frac{\mathrm{I}^\alpha(T_j - v_j)}{\mathrm{I}^\alpha(T_j)} \begin{cases} = \frac{1}{\alpha+1} & |T_j| = 1, \\ = \frac{\alpha+1}{2\alpha+1} & |T_j| = 2, \\ = \frac{2\alpha+1}{\alpha^2+3\alpha+1} & |T_j| = 3 \text{ and } v_j \text{ is a leaf of } T_j, \\ = \frac{\alpha^2+2\alpha+1}{\alpha^2+3\alpha+1} & |T_j| = 3 \text{ and } v_j \text{ is the centre of } T_j, \\ \in [\frac{1}{\alpha+1}, 1] & \text{otherwise}. \end{cases}$$

We plug these estimates into (4.2.6) and also use the identity (4.2.4) again. Since the expression (4.2.6) is linear in ρ_α, its minimum is either attained for the largest or smallest possible value of ρ_α. This gives us a lower bound for $\operatorname{avi}^\alpha(T)$ in each of the aforementioned 105 cases, which can all be checked with a computer. As an example, let us consider the case that gives us the worst estimate: it is obtained for $x_1 = x_3 = x_4 = x_5 = 0$ and $x_2 = 3$. Let T_i be a tree of two vertices for all i. We have for all i:

$$\operatorname{avi}^\alpha(T_i) = a|T_i| + c_2(\alpha)$$

and

$$\operatorname{avi}^\alpha(T_i - v_i) = a|T_i| + c_1(\alpha) - a,$$

as well as

$$\rho_\alpha = \frac{1}{1 + \alpha\left(\frac{\alpha+1}{2\alpha+1}\right)^3}.$$

Thus

$$\operatorname{avi}^\alpha(T_1) + \operatorname{avi}^\alpha(T_2) + \operatorname{avi}^\alpha(T_3) = a|T| + 3c_2(\alpha) - a.$$

and likewise

$$\operatorname{avi}^\alpha(T_1 - v_1) + \operatorname{avi}^\alpha(T_2 - v_2) + \operatorname{avi}^\alpha(T_3 - v_3) = a|T| + 3c_1(\alpha) - 4a.$$

Putting everything together, we obtain

$$\begin{aligned}
\operatorname{avi}^\alpha(T) &= \rho_\alpha\Big(a|T| + 3c_2(\alpha) - a\Big) + (1-\rho_\alpha)\Big(1 + a|T| + 3c_1(\alpha) - 4a\Big) \\
&= a|T| + \rho_\alpha\Big(3c_2(\alpha) - a\Big) + (1-\rho_\alpha)\Big(1 + 3c_1(\alpha) - 4a\Big) \\
&\geq a|T| + c_5(\alpha).
\end{aligned}$$

The worst case is drawn with a green color in Figure 4.3, other cases are treated in the same fashion.

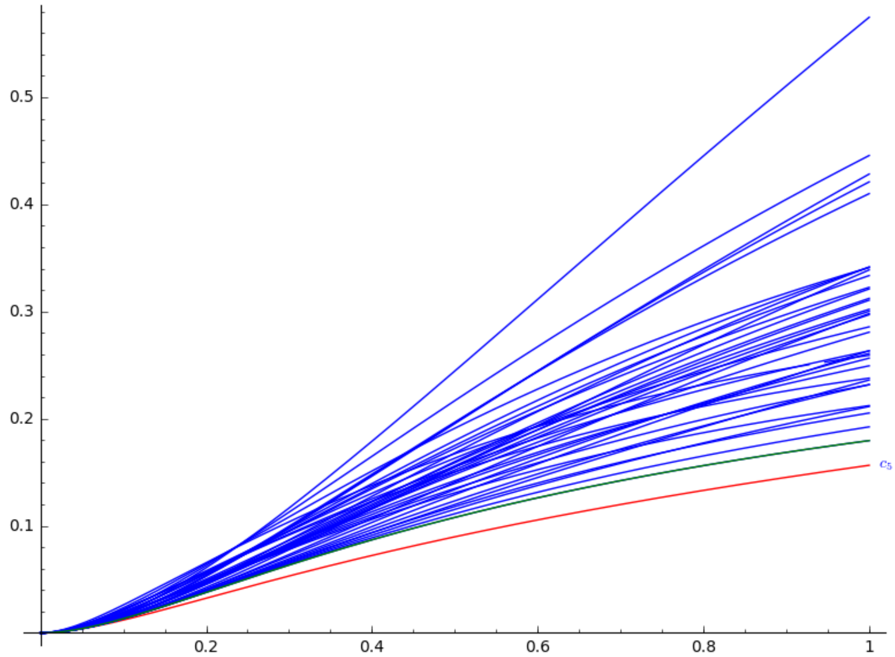


Figure 4.3: The 35 cases when $k = 3$.

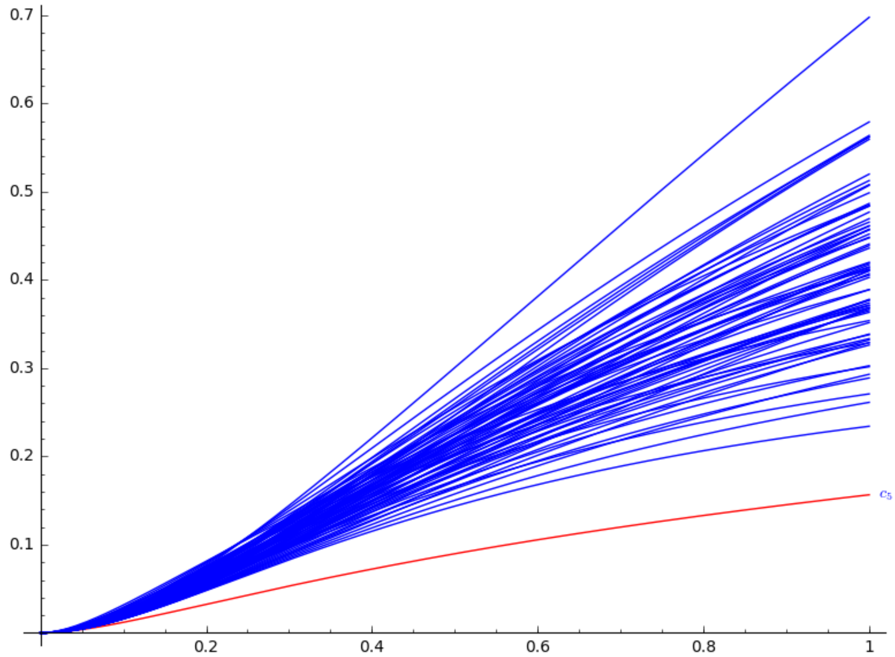


Figure 4.4: The 70 cases when $k = 4$.

To complete the proof of the theorem, it only remains to prove an upper bound on $\mathrm{avi}^{\alpha}(P_n)$. However, we already know from Lemma 4.2.4 that $\mathrm{avi}^{\alpha}(P_n) \leq an + c_5(\alpha)$, for $n > 3$. Thus $\mathrm{avi}^{\alpha}(P_n) \leq a|T| + c_5(\alpha) \leq \mathrm{avi}^{\alpha}(T)$ for every tree T with n vertices other than P_n. This completes the proof. ■

Theorems 4.2.3 and 4.2.6 give us the following corollary:

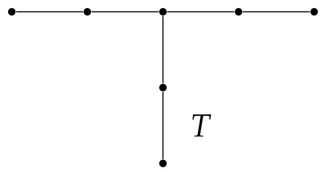
Corollary 4.2.7. *[52] For every n-vertex tree T,*

$$I(P_n) \leq \mathrm{I}(T) \leq \mathrm{I}(S_n).$$

Proof. In fact $\int_0^1 \frac{\mathrm{avi}^{\alpha}(T)}{\alpha} d\alpha = \log \mathrm{I}(G)$. Thus, the extremal trees for the weighted average size of independents sets are also extremal for the number of independent sets. ■

Unfortunately, Theorem 4.2.6 is no longer true for $\alpha > 1$. As a counterexample, let us consider trees of order 7.

Considering the following tree:



We have:

$$\mathrm{avi}^{\alpha}(T) = \frac{4\alpha^4 + 33\alpha^3 + 30\alpha^2 + 7\alpha}{\alpha^4 + 11\alpha^3 + 15\alpha^2 + 7\alpha + 1},$$
$$\mathrm{avi}^{\alpha}(P_7) = \frac{4\alpha^4 + 30\alpha^3 + 30\alpha^2 + 7\alpha}{\alpha^4 + 10\alpha^3 + 15\alpha^2 + 7\alpha + 1},$$

and $\mathrm{avi}^5(T) \approx 3.073413 < \mathrm{avi}^5(P_7) \approx 3.077427$.

When $\alpha > 1$, the tree which minimizes the weighted average size of independent sets changes depending on the order of the tree and the actual α. We are interested in what happens if α tends to infinity.

Let κ be the maximum size of the independent sets in T. Then

$$\mathrm{I}^{\alpha}(T) = \sum_{k \geq 0} \mathrm{i}(k,T)\alpha^k = 1 + \cdots + \mathrm{i}(\kappa-1,T)\alpha^{\kappa-1} + \mathrm{i}(\kappa,T)\alpha^{\kappa},$$
$$\mathrm{T}^{\alpha}(T) = \sum_{k \geq 0} k\,\mathrm{i}(k,T)\alpha^k = \mathrm{i}(1,T)\alpha + \cdots + (\kappa-1)\,\mathrm{i}(\kappa-1,T)\alpha^{\kappa-1} + \kappa\,\mathrm{i}(\kappa,T)\alpha^{\kappa}.$$

Thus,

$$\operatorname{avi}^{\alpha}(T) = \frac{\kappa\,\mathrm{i}(\kappa,T)\alpha^{\kappa} + (\kappa-1)\,\mathrm{i}(\kappa-1,T)\alpha^{\kappa-1} + \cdots + \mathrm{i}(1,T)\alpha}{\mathrm{i}(\kappa,T)\alpha^{\kappa} + \mathrm{i}(\kappa-1,T)\alpha^{\kappa-1} + \cdots + 1} \tag{4.2.7}$$

When $\alpha \to \infty$, we get from Equation (4.2.7) that

$$\begin{aligned}\operatorname{avi}^{\alpha}(T) &= \frac{\kappa\,\mathrm{i}(\kappa,T) + (\kappa-1)\,\mathrm{i}(\kappa-1,T)\alpha^{-1} + \cdots + \mathrm{i}(1,T)\alpha^{1-\kappa}}{\mathrm{i}(\kappa,T) + \mathrm{i}(\kappa-1,T)\alpha^{-1} + \cdots + \alpha^{-\kappa}} \\ &\to \kappa.\end{aligned} \tag{4.2.8}$$

So for sufficiently large α, the tree that minimizes $\operatorname{avi}^{\alpha}(T)$ has to have the smallest possible κ. Furthermore, if we multiply both numerator and denominator by $\mathrm{i}(\kappa,T) - \mathrm{i}(\kappa-1,T)\alpha^{-1}$ in Equation (4.2.8), we obtain

$$\begin{aligned}\operatorname{avi}^{\alpha}(T) &= \frac{\kappa\,\mathrm{i}(\kappa,T)^2 - \mathrm{i}(\kappa,T)\,\mathrm{i}(\kappa-1,T)\alpha^{-1} + \mathcal{O}(\alpha^{-2})}{\mathrm{i}(\kappa,T)^2 + \mathcal{O}(\alpha^{-2})}, \\ &= \kappa - \frac{\mathrm{i}(\kappa-1,T)}{\mathrm{i}(\kappa,T)}\alpha^{-1} + \mathcal{O}(\alpha^{-2}).\end{aligned}$$

Hence, the "optimal" tree should also maximize $\frac{\mathrm{i}(\kappa-1,T)}{\mathrm{i}(\kappa,T)}$ for large enough α.

Proposition 4.2.8. *Let κ be the maximum size of the independent sets in T. For large enough α, the tree T that minimizes $\operatorname{avi}^{\alpha}(T)$ has to have minimum κ and among all trees with this property maximum $\frac{\mathrm{i}(\kappa-1,T)}{\mathrm{i}(\kappa,T)}$.*

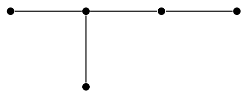
We say that a tree minimizes the average size of independent sets at "infinity" if it minimizes $\operatorname{avi}^{\alpha}(T)$ for sufficiently large α.

Theorem 4.2.9. *Among trees of order $n \leq 5$, the path P_n minimizes the average size of independent sets at infinity.*

Proof.

- For $n \leq 3$, there is nothing to prove since the only trees of three or fewer vertices are paths.
- For $n = 4$, the trees of this order are the path P_4 and the star S_4. We have already proved that S_4 is the one that maximizes the weighted average size of independent sets for any α.

- For $n = 5$, there are two trees that have minimum independence number 3, the path P_5 and the following tree T



T

However, $\mathrm{i}(3, P_5) = 1$, $\mathrm{i}(2, P_5) = 6$ and $\mathrm{i}(3, T) = 2$, $\mathrm{i}(2, T) = 6$, so we get

$$\frac{\mathrm{i}(2, P_5)}{\mathrm{i}(3, P5)} = 6 > \frac{\mathrm{i}(2, T)}{\mathrm{i}(3, T)} = 3.$$

Thus by Proposition 4.2.8, the path minimizes avi^{α} at infinity.

■

Conjecture 4.2.10. Among trees of order $n \geq 6$,

- if n is even, then the path P_n minimizes the average size of independent sets at infinity,
- otherwise the starlike tree $S(2, 2, \ldots, 2)$ (see Definition 2.3.6) minimizes the average size of independent sets at infinity.

Chapter 5

The average size of matchings in a graph

Independent vertex sets and independent edge sets, also called matchings of a graph, are closely related. For the class of trees, Wagner [59] showed that the total number of these sets are correlated. It turns out in numerous cases that the graphs that minimize one maximize the other, [1, 16, 35, 54, 68, 76]. However, there are some counterexamples for instance in [60]. For more articles related to extremal questions on the number of matchings of a graph, we may refer to [14, 15, 25, 26, 34, 44, 69, 70]. Analogously to Chapter 4, this chapter concerns the study of the average size of matchings in a graph. Explicitly, we characterize extremal graphs regarding to this parameter. Besides, we investigate also the connection between the average size of matchings and the matching energy of a graph, an invariant introduced in [30].

5.1 The average size of matchings in a graph

5.1.1 Preliminaries

Let G be a graph. A subset A of $E(G)$ is called a matching of G if the edges of A do not share common vertices. Let $\mathrm{m}(G,k)$ be the number of matchings of size k in G. We define the total number of matchings in G, the sum of the sizes of all matchings in G with their size and the average size of matchings in G as follows:

$$\mathrm{M}(G) = \sum_{k\geq 0} \mathrm{m}(G,k),$$
$$\mathrm{S}(G) = \sum_{k\geq 0} k\,\mathrm{m}(G,k),$$
$$\mathrm{av}(G) = \frac{\mathrm{S}(G)}{\mathrm{M}(G)}.$$

Similarly, let us define the following partial sums:

$$\mathrm{S}_k(G) = \sum_{i=0}^{k} i\,\mathrm{m}(G,i),$$
$$\mathrm{M}_k(G) = \sum_{i=0}^{k} \mathrm{m}(G,i),$$
$$\mathrm{av}_k(G) = \frac{S_k(G)}{\mathrm{M}_k(G)}.$$

Note that the largest size of a matching in G is called the matching number of G and denoted by $\mu(G)$.

As examples, let us consider the n-vertex edgeless graph E_n and star S_n. We have

$$\mathrm{M}(E_n) = 1, \quad \mathrm{M}(S_n) = n, \quad \mathrm{S}(E_n) = 0, \quad \mathrm{S}(S_n) = n-1$$

and hence

$$\mathrm{av}(E_n) = 0, \quad \mathrm{av}(S_n) = \frac{n-1}{n}.$$

From Propositions 2.4.6 and 2.4.7, we can obtain some recursive relations for M and S by plugging in $x = 1$.

If $e = uv$ is an edge of G, then

$$\mathrm{M}(G) = \mathrm{M}(G-e) + \mathrm{M}(G-v-u). \tag{5.1.1}$$

Similarly, if v is a vertex of G, then

$$\mathrm{M}(G) = \mathrm{M}(G-v) + \sum_{u:uv\in E(G)} \mathrm{M}(G-v-u). \tag{5.1.2}$$

In particular, if v is a leaf, we retrieve the same relation as for independent subsets of G.

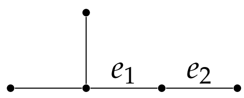
Now, by summing up the cardinality of matchings not containing e first and then the cardinality of those which contain e and use Equation (5.1.1), we obtain:

$$\mathrm{S}(G) = \mathrm{S}(G-e) + \mathrm{S}(G-v-u) + \mathrm{M}(G-v-u). \tag{5.1.3}$$

5.1.2 Edge removal

Unlike M, av is not always a monotone function under addition of an edge to the graph.

Considering the graph



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we get

$$\mathrm{av}(T - e_1) = \frac{7}{6} > \frac{8}{7} = \mathrm{av}(T), \text{ and } \mathrm{av}(T - e_2) = \frac{3}{4} < \mathrm{av}(T).$$

Theorem 5.1.1. *If G is a nonempty graph, then there exists an edge e in $E(G)$ such that*

$$\mathrm{av}(G - e) < \mathrm{av}(G).$$

Proof. Apply Theorem 4.1.3, with $\mathcal{B}$ being the set of matchings G. ∎

Corollary 5.1.2. *For any n-vertex graph G which is not the edgeless graph E_n, $0 = \mathrm{av}(E_n) < \mathrm{av}(G)$.*

Despite the fact that adding an edge does not necessarily increase the average size of matchings, we are going to show that the complete graph is still extremal. For this purpose, we will need the following lemmas.

Lemma 5.1.3. *For any integer $k \geq 0$ and any graph G, we have*

$$\mathrm{av}_{k+1}(G) \geq \mathrm{av}_k(G).$$

If $k \geq \mu(G)$, then

$$\mathrm{av}_{k+1}(G) = \mathrm{av}_k(G) = \mathrm{av}(G).$$

Proof. This is straightforward from the definition of av_k. ∎

Lemma 5.1.4. *For any n-vertex graph G and any integer $k \geq 0$, we have*

$$\frac{\mathrm{m}(K_n, k)}{\mathrm{m}(K_n, k+1)} \leq \frac{\mathrm{m}(G, k)}{\mathrm{m}(G, k+1)},$$

with equality only if $K_n = G$.

Proof. Note that if
$$N = \{\{u_i, v_i\} : i = 1, 2, \ldots, k\}$$
is a k-matching in G, then there are

$$|E(G - u_1 - v_1 - u_2 - v_2 - \cdots - u_k - v_k)|$$

ways to extend it to a $(k+1)$-matching.

If
$$L = \{\{z_i, s_i\} : i = 1, 2, \ldots, k\}$$
is a k-matching in K_n, then $K_n - z_1 - s_1 - z_2 - s_2 - \cdots - z_k - s_k$ is also a complete graph, and thus

$$\begin{aligned} &|E(G - u_1 - v_1 - u_2 - v_2 - \cdots - u_k - v_k)| \\ &\leq |E(K_n - z_1 - s_1 - z_2 - s_2 - \cdots - z_k - s_k)|, \end{aligned}$$

with equality if and only if $G - u_1 - v_1 - u_2 - v_2 - \cdots - u_k - v_k$ is also a complete graph.

(Note that $|E(K_n - z_1 - s_1 - z_2 - s_2 - \cdots - z_k - s_k)|$ is the same for any k-matching). ■

Lemma 5.1.4 can easily be extended to the following lemma:

Lemma 5.1.5. *For any graph G and for any integers $\mu(G) \geq k > l \geq 0$ we have*
$$\frac{\mathrm{m}(K_n, l)}{\mathrm{m}(K_n, k)} \leq \frac{\mathrm{m}(G, l)}{\mathrm{m}(G, k)}$$
and thus
$$\frac{\sum_{i=0}^{l} \mathrm{m}(K_n, i)}{\mathrm{m}(K_n, k)} \leq \frac{\sum_{i=0}^{l} \mathrm{m}(G, i)}{\mathrm{m}(G, k)},$$
with equality only if $G = K_n$.

Theorem 5.1.6. *For any n-vertex graph G and any $\mu(G) \geq k \geq 0$, we have*

$$\mathrm{av}_k(K_n) \geq \mathrm{av}_k(G),$$

with equality if and only if $G = K_n$.

Proof.
$$\mathrm{av}_0(K_n) = 0 = \mathrm{av}_0(G),$$

and
$$\mathrm{av}_1(K_n) = \frac{|E(K_n)|}{|E(K_n)|+1} \geq \frac{|E(G)|}{|E(G)|+1} = \mathrm{av}_1(G).$$
The last inequality holds because $\frac{x}{x+1}$ is an increasing function of $x \in [0, \infty)$.

Assume that $\mathrm{av}_k(K_n) \geq \mathrm{av}_k(G)$ for some $\mu(G) > k \geq 1$. Then we have $\mathrm{m}(k+1, G) \neq 0$ and

$$\begin{aligned}
\mathrm{av}_{k+1}(K_n) &= \frac{(k+1)\,\mathrm{m}(K_n, k+1) + \sum_{i=0}^{k} i\,\mathrm{m}(K_n, i)}{\mathrm{m}(K_n, k+1) + \sum_{i=0}^{k} \mathrm{m}(K_n, i)} \\
&= \frac{(k+1)\,\mathrm{m}(K_n, k+1) + \mathrm{S}_k(K_n)}{\mathrm{m}(K_n, k+1) + \mathrm{M}_k(K_n)} \\
&= \frac{(k+1)\,\mathrm{m}(K_n, k+1) + \mathrm{av}_k(K_n)\,\mathrm{M}_k(K_n)}{\mathrm{m}(K_n, k+1) + \mathrm{M}_k(K_n)} \\
&= \frac{(k+1) + \mathrm{av}_k(K_n)\frac{\mathrm{M}_k(K_n)}{\mathrm{m}(K_n,k+1)}}{1 + \frac{\mathrm{M}_k(K_n)}{\mathrm{m}(K_n,k+1)}}. \qquad (5.1.4)
\end{aligned}$$

Since $k+1 > \mathrm{av}_k(K_n)$, $\frac{k+1+\mathrm{av}_k(K_n)x}{1+x}$ is a decreasing function of $x \in [0, \infty)$, so Lemma 5.1.5 and (5.1.4) imply that

$$\mathrm{av}_{k+1}(K_n) \geq \frac{(k+1) + \mathrm{av}_k(K_n)\frac{\mathrm{M}_k(G)}{\mathrm{m}(G,k+1)}}{1 + \frac{\mathrm{M}_k(G)}{\mathrm{m}(G,k+1)}}. \qquad (5.1.5)$$

Furthermore, with the induction hypothesis $\mathrm{av}_k(K_n) \geq \mathrm{av}_k(G)$, we obtain

$$\mathrm{av}_{k+1}(K_n) \geq \frac{(k+1) + \mathrm{av}_k(G)\frac{\mathrm{M}_k(G)}{\mathrm{m}(G,k+1)}}{1 + \frac{\mathrm{M}_k(G)}{\mathrm{m}(G,k+1)}} = \mathrm{av}_{k+1}(G). \qquad (5.1.6)$$

■

Corollary 5.1.7. *For any n-vertex graph G we have* $\mathrm{av}(K_n) \geq \mathrm{av}(G)$, *with equality only if $G = K_n$.*

Proof. By Theorem 5.1.6 and Lemma 5.1.3 we get

$$\mathrm{av}(K_n) = \mathrm{av}_{\lfloor n/2 \rfloor}(K_n) \geq \mathrm{av}_{\mu(G)}(K_n) \geq \mathrm{av}_{\mu(G)}(G) = \mathrm{av}(G).$$

■

5.1.3 The case of trees

Let us first consider the problem on the minimization of the average size of matchings.

Theorem 5.1.8. *For any connected n-vertex tree $G \neq S_n$, $\mathrm{av}(S_n) < \mathrm{av}(G)$.*

Proof. We have shown earlier that $\mathrm{av}(S_n) = \frac{n-1}{n} < 1$. However any other tree T on n vertices satisfies $\mathrm{av}(T) \geq 1$, since T possesses matchings of size greater or equal to 2, which balances with the empty set.

∎

The maximization requires more techniques. Note that the line graph of the n-vertex path P_n is the $(n-1)$-vertex path P_{n-1}. This implies that the matchings of P_n can be identified with the independent sets of P_{n-1}. Thus, the average size of matchings of P_n ($\mathrm{av}(P_n)$) is the same as the average size of the independent sets of P_{n-1} ($\mathrm{avi}(P_{n-1})$). Using the same approach as for independent sets, let us find an explicit formula for the average size of matchings of a path.

Lemma 5.1.9. *The average size of matchings of the n-vertex path P_n is*

$$\mathrm{av}(P_n) = \mathrm{avi}(P_{n-1}) = \frac{5-\sqrt{5}}{10}n + \frac{1-\sqrt{5}}{10} - \frac{n+1}{\sqrt{5}((-\phi^2)^{n+1}-1)}, \tag{5.1.7}$$

where $\phi = \frac{\sqrt{5}+1}{2}$ is the golden ratio. In particular,

(a) $\lim_{n\to\infty} \mathrm{av}(P_n) - \frac{5-\sqrt{5}}{10}n = \frac{1-\sqrt{5}}{10}$,

(b) $\mathrm{av}(P_n) \leq \frac{5-\sqrt{5}}{10}n + \frac{1}{\sqrt{5}} - \frac{1}{2}$, *with equality only for $n = 2$. For all positive integers $n \neq 2$, we even have* $\mathrm{av}(P_n) \leq \frac{5-\sqrt{5}}{10}n + \frac{2}{\sqrt{5}} - 1$.

For ease of notation, we set $a = \frac{5-\sqrt{5}}{10} \approx 0.27639320$ and $c_n = \mathrm{av}(P_n) - an$. Table 5.1 gives values of c_n for small n.

Before we prove our result, we require one more lemma:

Lemma 5.1.10. *For every tree T and every vertex v of T, we have*

$$\frac{1}{1+d(v)} \leq \frac{\mathrm{M}(T-v)}{\mathrm{M}(T)} < 1.$$

n	1	2	3
c_n	$\frac{-5+\sqrt{5}}{10} \approx -0.2764$	$\frac{1}{\sqrt{5}} - \frac{1}{2} \approx -0.0527$	$\frac{3}{2\sqrt{5}} - \frac{5}{6} \approx -0.1625$

n	4	5
c_n	$\frac{2}{\sqrt{5}} - 1 \approx -0.1055$	$\frac{\sqrt{5}}{2} - \frac{5}{4} \approx -0.1319$

Table 5.1: Values of $c_1, c_2, \ldots, c_5$ for matchings.

Proof. Note first that $\mathrm{M}(T) = \mathrm{M}(T-v) + \sum_{uv \in E(T)}(T-v-u)$. Since $T - v - u$ is a subgraph of $T - v$, we have $\mathrm{M}(T-v-u) \leq \mathrm{M}(T-v)$, hence $(1+d(v))\,\mathrm{M}(T-v) \geq \mathrm{M}(T)$, which proves the first inequality. The second inequality simply follows from the fact that $T - v$ is a proper subgraph of T. ■

Theorem 5.1.11. *For every tree T of order n that is not a path, we have the inequality $\mathrm{av}(T) \leq an + b$, where $b = (7\sqrt{5} - 17)/10 \approx -0.13475241$. Consequently, the path maximises the value of $\mathrm{av}(T)$ among all trees of order n.*

Proof. We prove the inequality by induction on n. For $n \leq 3$, there is nothing to prove since the only trees with three or fewer vertices are paths. Thus assume now that $n \geq 4$, and consider a vertex v of the tree T whose degree is at least 3 (which must exist if T is not a path). Denote the neighbours of v by $v_1, v_2, \ldots, v_k$ and the components of $T - v$ by $T_1, T_2, \ldots, T_k$ (in such a way that v_j is contained in T_j). Let e be the edge between v and v_k, and $T' = T - T_k$ be the tree obtained by removing T_k from T. We have

$$\begin{aligned}
\mathrm{av}(T) &= \frac{\mathrm{S}(T)}{\mathrm{M}(T)} = \frac{\mathrm{S}(T-e) + \mathrm{S}(T-v-v_k) + \mathrm{M}(T-v-v_k))}{\mathrm{M}(T)} \\
&= \frac{\mathrm{M}(T-e)}{\mathrm{M}(T)} \cdot \frac{\mathrm{S}(T-e)}{\mathrm{M}(T-e)} + \frac{\mathrm{M}(T-v-v_k)}{\mathrm{M}(T)} \cdot \Big(1 + \frac{\mathrm{S}(T-v-v_k)}{\mathrm{M}(T-v-v_k)}\Big) \\
&= \frac{\mathrm{M}(T-e)}{\mathrm{M}(T)} \mathrm{av}(T-e) + \frac{\mathrm{M}(T) - \mathrm{M}(T-e)}{\mathrm{M}(T)} (1 + \mathrm{av}(T-v-v_k)) \\
&= \frac{\mathrm{M}(T-e)}{\mathrm{M}(T)} (\mathrm{av}(T') + \mathrm{av}(T_k)) \\
&\quad + \Big(1 - \frac{\mathrm{M}(T-e)}{\mathrm{M}(T)}\Big)\Big(1 + \sum_{j=1}^{k-1} \mathrm{av}(T_j) + \mathrm{av}(T_k - v_k)\Big) \\
&= \frac{\mathrm{M}(T-e)}{\mathrm{M}(T)} A + \Big(1 - \frac{\mathrm{M}(T-e)}{\mathrm{M}(T)}\Big) B.
\end{aligned}$$

Assume first that $k \geq 4$. By Lemma 5.1.9 and the induction hypothesis, we have $\mathrm{av}(T_j) \leq a|T_j| + \frac{1}{\sqrt{5}} - \frac{1}{2}$ for all j and $\mathrm{av}(T') \leq a|T'| + b$. It follows that

$$A \leq a(|T'| + |T_k|) + b + \frac{1}{\sqrt{5}} - \frac{1}{2} < a|T| + b.$$

If $B \leq a|T| + b$, then we are done. Hence we can assume $A < a|T| + b \leq B$. This implies that $\mathrm{av}(T)$ is now decreasing regarded as a function of $\frac{\mathrm{M}(T-e)}{\mathrm{M}(T)}$. So let us find an explicit formula for $\frac{\mathrm{M}(T-e)}{\mathrm{M}(T)}$. We observe that:

$$\frac{\mathrm{M}(T-e)}{\mathrm{M}(T)} = \frac{\mathrm{M}(T')\,\mathrm{M}(T_k)}{\mathrm{M}(T')\,\mathrm{M}(T_k) + \mathrm{M}(T'-v)\,\mathrm{M}(T_k - v_k)},$$

thus

$$\frac{\mathrm{M}(T-e)}{\mathrm{M}(T)} = \frac{1}{1 + \frac{\mathrm{M}(T'-v)}{\mathrm{M}(T')} \cdot \frac{\mathrm{M}(T_k - v_k)}{\mathrm{M}(T_k)}}. \tag{5.1.8}$$

Let us find an explicit formula for $\frac{\mathrm{M}(T'-v)}{\mathrm{M}(T')}$.

$$\begin{aligned}\frac{\mathrm{M}(T'-v)}{\mathrm{M}(T')} &= \frac{\prod_j^{k-1} \mathrm{M}(T_j)}{\prod_j^{k-1} \mathrm{M}(T_j) + \sum_j^{k-1} \frac{\prod_j^{k-1} \mathrm{M}(T_j)}{\mathrm{M}(T_j)} \cdot \mathrm{M}(T_j - v_j)} \\ &= \frac{1}{1 + \sum_j^{k-1} \frac{\mathrm{M}(T_j - v_j)}{\mathrm{M}(T_j)}}. \end{aligned} \tag{5.1.9}$$

Two cases can be considered:

Case 1: One of the T_j's is P_2. Then we can without loss of generality assume that $T_k = P_2$. Let us observe two subcases depending on the number of P_2's among the branches T_j.

- at least one of the T_j's is different from P_2. Then by Lemma 5.1.9 and the induction hypothesis

$$\begin{aligned} A &\leq a|T| + b + \frac{1}{\sqrt{5}} - \frac{1}{2}, \\ B &\leq 1 + a(|T'| - 1) + 2\left(\frac{1}{\sqrt{5}} - \frac{1}{2}\right) + \frac{2}{\sqrt{5}} - 1 + a|T_k| - 2a \\ &= a|T| - 3a + \frac{4}{\sqrt{5}} - 1. \end{aligned}$$

Moreover, from Lemma 5.1.10, $\frac{\mathrm{M}(T'-v)}{\mathrm{M}(T')} \leq 1$, and the fact that $\frac{\mathrm{M}(T_k-v_k)}{\mathrm{M}(T_k)} = \frac{1}{2}$, so using Equation (5.1.8), we obtain $\frac{\mathrm{M}(T-e)}{\mathrm{M}(T)} \geq \frac{2}{3}$. Hence

$$\begin{aligned} \mathrm{av}(T) &\leq a|T| + \frac{2}{3}\left(b + \frac{1}{\sqrt{5}} - \frac{1}{2}\right) + \frac{1}{3}\left(-3a + \frac{4}{\sqrt{5}} - 1\right) \\ &= a|T| + \frac{29}{6\sqrt{5}} - \frac{23}{10} \approx a|T| - 0.13847 < a|T| + b. \end{aligned}$$

- all of the T_j's are equal to P_2. Then by Lemma 5.1.9 and the induction hypothesis

$$\begin{aligned} A &\leq a|T| + b + \frac{1}{\sqrt{5}} - \frac{1}{2}, \\ B &\leq 1 + a(|T'| - 1) + 3\left(\frac{1}{\sqrt{5}} - \frac{1}{2}\right) + a|T_k| - 2a \\ &= a|T| + 1 - 3a + 3\left(\frac{1}{\sqrt{5}} - \frac{1}{2}\right). \end{aligned}$$

Equation (5.1.9) gives us the following estimation:

$$\begin{aligned} \frac{\mathrm{M}(T'-v)}{\mathrm{M}(T')} &= \frac{1}{1 + \sum_j^{k-1} \frac{\mathrm{M}(T_j - v_j)}{\mathrm{M}(T_j)}} \\ &= \frac{1}{1 + (k-1)\frac{1}{2}} \leq \frac{1}{1 + \frac{3}{2}} = \frac{2}{5}. \end{aligned}$$

Plugging these estimates into Equation (5.1.8), we have

$$\frac{\mathrm{M}(T-e)}{\mathrm{M}(T)} \geq \frac{1}{1 + \frac{2}{5}\cdot\frac{1}{2}} = \frac{5}{6}.$$

Thus,

$$\begin{aligned} \mathrm{av}(T) &\leq a|T| + \frac{5}{6}\left(b + \frac{1}{\sqrt{5}} - \frac{1}{2}\right) + \frac{1}{6}\left(1 - 3a + 3\left(\frac{1}{\sqrt{5}} - \frac{1}{2}\right)\right) \\ &= a|T| + \frac{9}{2\sqrt{5}} - \frac{13}{6} \approx a|T| - 0.1542 < a|T| + b. \end{aligned}$$

Case 2: None of the T_j's is P_2.

By Lemma 5.1.10, $\frac{\mathrm{M}(T'-v)}{\mathrm{M}(T')} \leq 1$, and plugging this estimate in Equation (5.1.8), we obtain

$$\frac{\mathrm{M}(T-e)}{\mathrm{M}(T)} \geq \frac{1}{1 + \frac{\mathrm{M}(T_k - v)}{\mathrm{M}(T_k)}}. \tag{5.1.10}$$

Let us distinguish different cases depending on T_k. We may assume that $|T_k| = \min_{1\le j\le k} |T_j|$.

- If $|T_k| = 1$, then $\mathrm{av}(T_k) = \mathrm{av}(T_k - v_k) = 0 = a|T_k| - a$. It follows that

$$\begin{aligned} A &\le a|T'| + b + a|T_k| - a = a|T| + b - a, \\ B &\le 1 + a|T'| + 3\left(\frac{2}{\sqrt{5}} - 1\right) - a + a|T_k| - a \\ &= a|T| + 1 - 2a + 3\left(\frac{2}{\sqrt{5}} - 1\right). \end{aligned}$$

Since $\frac{\mathrm{M}(T_k - v)}{\mathrm{M}(T_k)} = 1$, Equation (5.1.10) gives us $\frac{\mathrm{M}(T-e)}{\mathrm{M}(T)} \ge \frac{1}{2}$. Thus,

$$\begin{aligned} \mathrm{av}(T) &\le \frac{1}{2}(a|T| + b - a) + \frac{1}{2}\left(a|T| + 1 - 2a + 3\left(\frac{2}{\sqrt{5}} - 1\right)\right) \\ &= a|T| + \frac{1}{2}\left(b + 1 - 3a + 3\left(\frac{2}{\sqrt{5}} - 1\right)\right) \\ &= a|T| + \frac{11}{2\sqrt{5}} - \frac{13}{5} \approx a|T| - 0.14032 \le a|T| + b. \end{aligned}$$

- If $|T_k| = 3$, then $\mathrm{av}(T_k) = a|T_k| + \frac{3}{2\sqrt{5}} - \frac{5}{6}$ and $\mathrm{av}(T_k - v_k) \le a|T_k| - a + \frac{1}{\sqrt{5}} - \frac{1}{2}$. It follows that

$$\begin{aligned} A &\le a|T| + b + \frac{3}{2\sqrt{5}} - \frac{5}{6}, \\ B &\le 1 + a|T'| + 3\left(\frac{2}{\sqrt{5}} - 1\right) - a + a|T_k| - a + \frac{1}{\sqrt{5}} - \frac{1}{2} \\ &= a|T| - 2a + \frac{7}{\sqrt{5}} - \frac{5}{2}. \end{aligned}$$

Since $\frac{\mathrm{M}(T_k) - v_k}{\mathrm{M}(T_k)} \le \frac{2}{3}$, by Equation (5.1.10) $\frac{\mathrm{M}(T-e)}{\mathrm{M}(T)} \ge \frac{3}{5}$. We obtain

$$\begin{aligned} \mathrm{av}(T) &\le a|T| + \frac{3}{5}\left(b + \frac{3}{2\sqrt{5}} - \frac{5}{6}\right) + \frac{2}{5}\left(-2a + \frac{7}{\sqrt{5}} - \frac{5}{2}\right) \\ &= a|T| + \frac{31}{5\sqrt{5}} - \frac{73}{25} \approx a|T| - 0.14727 \le a|T| + b. \end{aligned}$$

- If $|T_k| = 4$, then $\mathrm{av}(T_k) \leq a|T_k| + \frac{2}{\sqrt{5}} - 1$ and $\mathrm{av}(T_k - v_k) \leq a|T_k| - a + \frac{3}{2\sqrt{5}} - \frac{5}{6}$. It follows that

$$\begin{aligned} A &\leq a|T| + b + \frac{2}{\sqrt{5}} - 1, \\ B &\leq 1 + a|T'| + 3\left(\frac{2}{\sqrt{5}} - 1\right) - a + a|T_k| - a + \frac{3}{2\sqrt{5}} - \frac{5}{6} \\ &= a|T| - 2a + \frac{15}{2\sqrt{5}} - \frac{17}{6}. \end{aligned}$$

Moreover, $\frac{\mathrm{M}(T_k) - v_k}{\mathrm{M}(T_k)} \leq \frac{3}{4}$, so using Equation (5.1.10) again, we get $\frac{\mathrm{M}(T-e)}{\mathrm{M}(T)} \geq \frac{4}{7}$. Hence

$$\begin{aligned} \mathrm{av}(T) &\leq a|T| + \frac{4}{7}\left(b + \frac{2}{\sqrt{5}} - 1\right) + \frac{3}{7}\left(-2a + \frac{15}{2\sqrt{5}} - \frac{17}{6}\right) \\ &= a|T| + \frac{95}{14\sqrt{5}} - \frac{669}{210} \approx a|T| - 0.15105 \leq a|T| + b. \end{aligned}$$

- If $|T_k| \geq 5$, then $\mathrm{av}(T_j) \leq a|T_j| + \frac{3}{\sqrt{5}} - \frac{19}{13}$ for all j and $\mathrm{av}(T_k - v_k) \leq a|T_k| - a + \frac{2}{\sqrt{5}} - 1$. It follows that

$$\begin{aligned} A &\leq a|T| + b + \frac{3}{\sqrt{5}} - \frac{19}{13}, \\ B &\leq 1 + a|T'| + 3\left(\frac{3}{\sqrt{5}} - \frac{19}{13}\right) - a + a|T_k| - a + \frac{2}{\sqrt{5}} - 1 \\ &= a|T| - 2a + 3\left(\frac{3}{\sqrt{5}} - \frac{19}{13}\right) + \frac{2}{\sqrt{5}}. \end{aligned}$$

Since $\frac{\mathrm{M}(T_k - v_k)}{\mathrm{M}(T_k)} \leq 1$, we have $\frac{\mathrm{M}(T-e)}{\mathrm{M}(T)} \geq \frac{1}{2}$. Thus,

$$\begin{aligned} \mathrm{av}(T) &\leq a|T| + \frac{1}{2}\left(b - 2a + 4\left(\frac{3}{\sqrt{5}} - \frac{19}{13}\right) + \frac{2}{\sqrt{5}}\right) \\ &= a|T| + \frac{37}{4\sqrt{5}} - \frac{1111}{260} \approx a|T| - 0.13635 \leq a|T| + b. \end{aligned}$$

This completes the case when $k \geq 4$, so we are left with the case $k = 3$. We return to the representation

$$\begin{aligned} \mathrm{av}(T) &= \frac{\mathrm{M}(T-e)}{\mathrm{M}(T)}(\mathrm{av}(T') + \mathrm{av}(T_k)) \\ &\quad + \left(1 - \frac{\mathrm{M}(T-e)}{\mathrm{M}(T)}\right)\left(1 + \sum_{j=1}^{k-1} \mathrm{av}(T_j) + \mathrm{av}(T_k - v_k)\right). \end{aligned} \tag{5.1.11}$$

Plugging (5.1.9) into Equation (5.1.8), we obtain

$$\frac{\mathrm{M}(T-e)}{\mathrm{M}(T)} = \frac{1}{1 + \frac{1}{1+\sum_j^{k-1} \frac{\mathrm{M}(T_j - v_j)}{\mathrm{M}(T_j)}} \cdot \frac{\mathrm{M}(T_k - v_k)}{\mathrm{M}(T_k)}}. \tag{5.1.12}$$

Now, let us distinguish different cases depending on how many of the branches T_j have one, two, three, four and five or more vertices respectively. This gives us a total of 35 cases corresponding to the solutions of

$$x_1 + x_2 + x_3 + x_4 + x_5 = 3.$$

Here, x_1, x_2, x_3, x_4 stand for the number of T_j's with one, two, three, four vertices respectively, and x_5 is the number of T_j's with five or more vertices. In each of the cases, we use the following explicit values and estimates:

$$\operatorname{av}(T_j) \begin{cases} = a|T_j| - a & |T_j| = 1, \\ = a|T_j| + c_2 & |T_j| = 2, \\ = a|T_j| + c_3 & |T_j| = 3, \\ \leq a|T_j| + c_4 & |T_j| = 4, \\ \leq a|T_j| + c_6 & \text{otherwise,} \end{cases}$$

$$\operatorname{av}(T_j - v_j) \begin{cases} = a|T_j| - a & |T_j| = 1, \\ = a|T_j| - 2a & |T_j| = 2, \\ \leq a|T_j| + c_2 - a & |T_j| = 3, \\ \leq a|T_j| + c_3 - a & |T_j| = 4, \\ \leq a|T_j| + c_4 - a & \text{otherwise.} \end{cases}$$

We can assume that the outdgree of v_j, which is its degree when removing v, is at most 2, since otherwise $d(v_j) \geq 4$ and we can go back to the previous cases. Using this assumption and Lemma 5.1.10, we have

$$\frac{\mathrm{M}(T_j - v_j)}{\mathrm{M}(T_j)} \begin{cases} = 1 & |T_j| = 1, \\ = \frac{1}{2} & |T_j| = 2, \\ \in [\frac{1}{3}, \frac{2}{3}] & |T_j| = 3, \\ \in [\frac{2}{5}, \frac{3}{4}] & |T_j| = 4, \\ \in [\frac{4}{11}, \frac{3}{4}] & \text{otherwise.} \end{cases}$$

We plug these estimates into (5.1.11) and also use the identity (5.1.12). Moreover, $\mathrm{av}(T') + \mathrm{av}(T_k) \leq a|T| + c_2 + c_4 < a|T| + b$. As before, if $1 + \sum_j^{k-1} \mathrm{av}(T_j)$ $+ \mathrm{av}(T_j - v_j) \leq a|T| + b$, then we are done. So we may assume $\mathrm{av}(T') +$ $\mathrm{av}(T_k) < a|T| + b \leq 1 + \sum_j^{k-1} \mathrm{av}(T_j) + \mathrm{av}(T_j - v_j)$. Hence the expression (5.1.11) is linear and decreasing in $\frac{\mathrm{M}(T-e)}{\mathrm{M}(T)}$, its maximum is attained for the smallest possible value of $\frac{\mathrm{M}(T-e)}{\mathrm{M}(T)}$. By the induction hypothesis, $\mathrm{av}(T') \leq \mathrm{av}(P_{|T'|})$. This gives us an upper bound for $a(T)$ in each of the aforementioned 35 cases, which can all be checked easily with a computer. The worst case is when $x_1 = x_3 = x_4 = x_5 = 0$ and $x_2 = 3$, where we have the equality $\mathrm{av}(T) = a|T| + b$. As another example, let us consider the case that gives us the second worst estimate: it is obtained for $x_1 = x_3 = x_5 = 0$, $x_2 = 2$ and $x_4 = 1$. Let T_1 and T_2 both have two vertices, so that the third branch T_3 consists of four vertices. We have

$$\mathrm{av}(T_1) = a|T_1| + c_2,\ \mathrm{av}(T') \leq a|T'| + c_7$$

and

$$\mathrm{av}(T_1 - v_1) = a|T_1| - 2a,\ \mathrm{av}(T_2) = a|T_2| + c_2,\ \mathrm{av}(T_3) \leq a|T_3| + c_4$$

as well as

$$\frac{\mathrm{M}(T-e)}{\mathrm{M}(T)} \geq \frac{1}{1 + \frac{1}{2}\frac{1}{1+\frac{1}{2}+\frac{2}{5}}} = \frac{19}{24}.$$

Thus

$$\begin{aligned}\mathrm{av}(T_1) + \mathrm{av}(T') &\leq a(|T_1| + |T'|) + c_2 + c_7 \\ &= a|T| + \frac{9}{2\sqrt{5}} - \frac{46}{21}\end{aligned}$$

and likewise

$$\begin{aligned}\mathrm{av}(T_1 - v_1) + \mathrm{av}(T_2) + \mathrm{av}(T_3) &\leq a(|T_1| + |T_2| + |T_3|) + c_2 + c_4 - 2a \\ &= a|T| + \frac{9}{2\sqrt{5}} - 3.\end{aligned}$$

Putting everything together, we obtain

$$\begin{aligned}\mathrm{av}(T) \leq & \frac{\mathrm{M}(T-e)}{\mathrm{M}(T)}\left(a|T| + \frac{9}{2\sqrt{5}} - \frac{46}{21}\right) \\ & + \left(1 - \frac{\mathrm{M}(T-e)}{\mathrm{M}(T)}\right)\left(1 + a|T| + \frac{9}{2\sqrt{5}} - 3\right) \\ \leq & \, a|T| + \frac{9}{2\sqrt{5}} - \frac{271}{126} \approx a|T| - 0.13833 < a|T| + b.\end{aligned}$$

The other cases are treated in the same fashion and give upper bounds with smaller constant terms. To complete the proof of the theorem, it only remains to prove an upper bound on $\mathrm{av}(P_n)$. However, we already know from Lemma 5.1.9 that

$$\begin{aligned}\mathrm{av}(P_n) &= an + \frac{1-\sqrt{5}}{10} - \frac{n+1}{\sqrt{5}((-\phi^2)^{n+1}-1)} \\ &\geq an + \frac{3-\sqrt{5}}{5} - \frac{6}{\sqrt{5}((-\phi^2)^6-1)} = an + \frac{\sqrt{5}}{2} - \frac{5}{4}\end{aligned}$$

for $n > 3$, and $\frac{\sqrt{5}}{2} - \frac{5}{4} \approx -0.131966 > b$. Thus $\mathrm{av}(P_n) > an + b \geq \mathrm{av}(T)$ for every tree T with n vertices other than P_n. This completes the proof. ∎

5.2 The weighted average size of matchings in a graph

As for independent sets, we may consider as well a probability distribution over matchings. This defines the monomer-dimer model from statistical physics [12]. This provides a motivation to our study of the weighted average size of matchings.

5.2.1 General considerations

Now, let us consider a random matching with probability proportional to α^k, where k is its size and α is a positive number. We define the weighted total number of matchings in G, the weighted total size of G and the weighted average size of matchings in G as follows:

$$\begin{aligned}\mathrm{M}^\alpha(G) &= \sum_{k\geq 0} \mathrm{m}(G,k)\alpha^k, \\ \mathrm{S}^\alpha(G) &= \sum_{k\geq 0} k\,\mathrm{m}(G,k)\alpha^k, \\ \mathrm{av}^\alpha(G) &= \frac{\mathrm{S}^\alpha(G)}{\mathrm{M}^\alpha(G)}.\end{aligned}$$

Similarly, let us define the following partial sums:

$$\begin{aligned} \mathrm{S}_k^\alpha(G) &= \sum_{i=0}^{k} i\,\mathrm{m}(G,i)\alpha^i, \\ \mathrm{M}_k^\alpha(G) &= \sum_{i=0}^{k} \mathrm{m}(G,i)\alpha^i, \\ \mathrm{av}_k^\alpha(G) &= \frac{S_k^\alpha(G)}{\mathrm{M}_k^\alpha(G)}. \end{aligned}$$

Theorem 5.2.1. *For any n-vertex graph G which is not the edgeless graph E_n, $0 = \mathrm{av}^\alpha(E_n) < \mathrm{av}^\alpha(G)$.*

Proof. This is trivial. ■

Lemma 5.2.2. *For any integer $k \geq 0$ and any graph G, we have*

$$\mathrm{av}_{k+1}^\alpha(G) \geq \mathrm{av}_k^\alpha(G).$$

If $k \geq \mu(G)$, then

$$\mathrm{av}_{k+1}^\alpha(G) = \mathrm{av}_k^\alpha(G) = \mathrm{av}^\alpha(G).$$

Proof. From the definition, we have

$$\begin{aligned} &\mathrm{av}_{k+1}^\alpha(G) - \mathrm{av}_k^\alpha(G) \\ &= \frac{\sum_{i=0}^k i\,\mathrm{m}(G,i)\alpha^i + (k+1)m(G,k+1)\alpha^{k+1}}{\sum_{i=0}^k \mathrm{m}(G,i)\alpha^i + m(G.k+1)\alpha^{k+1}} - \frac{\sum_{i=0}^k i\,\mathrm{m}(G,i)\alpha^i}{\sum_{i=0}^k \mathrm{m}(G,i)\alpha^i} \\ &= \frac{\left((k+1)\sum_{i=0}^k \mathrm{m}(G,i)\alpha^i - \sum_{i=0}^k i\,\mathrm{m}(G,i)\alpha^i\right)\mathrm{m}(G,k+1)\alpha^{k+1}}{\left(\sum_{i=0}^k \mathrm{m}(G,i)\alpha^i + m(G,k+1)\alpha^{k+1}\right)\left(\sum_{i=0}^k \mathrm{m}(i,G)\alpha^i\right)} \\ &\geq 0. \end{aligned}$$

The second part of the lemma is straightforward from the definition of av_k^α. ■

Lemma 5.1.5 can be extended as follows:

Lemma 5.2.3. *For any graph G and for any integers $\mu(G) \geq k > l \geq 0$ we have*

$$\frac{\mathrm{m}(K_n,l)\alpha^l}{\mathrm{m}(K_n,k)\alpha^k} \leq \frac{\mathrm{m}(G,l)\alpha^l}{\mathrm{m}(G,k)\alpha^k}$$

and thus

$$\frac{\sum_{i=0}^{l} \mathrm{m}(K_n,i)\alpha^i}{\mathrm{m}(K_n,k)\alpha^k} \leq \frac{\sum_{i=0}^{l} \mathrm{m}(G,i)\alpha^i}{\mathrm{m}(G,k)\alpha^k},$$

with equality only if $G = K_n$.

Theorem 5.2.4. *For any n-vertex graph G and any $\mu(G) \geq k \geq 0$, we have*

$$\mathrm{av}_k^\alpha(K_n) \geq \mathrm{av}_k^\alpha(G),$$

with equality if and only if $G = K_n$ or $k = 0$.

Proof.

$$\mathrm{av}_0^\alpha(K_n) = 0 = \mathrm{av}_0^\alpha(G),$$

and

$$\mathrm{av}_1^\alpha(K_n) = \frac{|E(K_n)|\alpha}{|E(K_n)|\alpha + 1} \geq \frac{|E(G)|\alpha}{|E(G)|\alpha + 1} = \mathrm{av}_1^\alpha(G).$$

The last inequality holds because $\frac{\alpha x}{\alpha x+1}$ is an increasing function of $x \in [0, \infty)$ since α is positive.

Assume that $\mathrm{av}_k^\alpha(K_n) \geq \mathrm{av}_k^\alpha(G)$ for some $\mu(G) > k \geq 1$. Then we have $\mathrm{m}(k+1, G) \neq 0$ and

$$\begin{aligned}
\mathrm{av}_{k+1}^\alpha(K_n) &= \frac{(k+1)\,\mathrm{m}(K_n,k+1)\alpha^{k+1} + \sum_{i=0}^{k} i\,\mathrm{m}(K_n,i)\alpha^i}{\mathrm{m}(K_n,k+1)\alpha^{k+1} + \sum_{i=0}^{k} \mathrm{m}(K_n,i)\alpha^i} \\
&= \frac{(k+1)\,\mathrm{m}(K_n,k+1)\alpha^{k+1} + \mathrm{S}_k^\alpha(K_n)}{\mathrm{m}(K_n,k+1)\alpha^{k+1} + \mathrm{M}_k(K_n)} \\
&= \frac{(k+1)\,\mathrm{m}(K_n,k+1)\alpha^{k+1} + \mathrm{av}_k^\alpha(K_n)\,\mathrm{M}_k(K_n)}{\mathrm{m}(K_n,k+1)\alpha^{k+1} + \mathrm{M}_k(K_n)} \\
&= \frac{(k+1) + \mathrm{av}_k^\alpha(K_n)\frac{\mathrm{M}_k(K_n)}{\mathrm{m}(K_n,k+1)\alpha^{k+1}}}{1 + \frac{\mathrm{M}_k^\alpha(K_n)}{\mathrm{m}(K_n,k+1)\alpha^{k+1}}}. \qquad (5.2.1)
\end{aligned}$$

Since $k+1 > \mathrm{av}_k^\alpha(K_n)$ and thus $\frac{k+1+\mathrm{av}_k^\alpha(K_n)x}{1+x}$ is a decreasing function of $x \in [0, \infty)$, Lemma 5.2.3 and (5.2.1) imply that

$$\mathrm{av}_{k+1}^\alpha(K_n) \geq \frac{(k+1) + \mathrm{av}_k^\alpha(K_n)\frac{\mathrm{M}_k^\alpha(G)}{\mathrm{m}(G,k+1)\alpha^{k+1}}}{1 + \frac{\mathrm{M}_k^\alpha(G)}{\mathrm{m}(G,k+1)\alpha^{k+1}}}. \qquad (5.2.2)$$

Furthermore, with the induction hypothesis $\mathrm{av}_k^\alpha(K_n) \geq \mathrm{av}_k^\alpha(G)^k$, we obtain

$$\mathrm{av}_{k+1}^\alpha(K_n) \geq \frac{(k+1) + \mathrm{av}_k^\alpha(G)\frac{\mathrm{M}_k^\alpha(G)}{\mathrm{m}(G,k+1)\alpha^{k+1}}}{1 + \frac{\mathrm{M}_k^\alpha(G)}{\mathrm{m}(G,k+1)\alpha^{k+1}}} = \mathrm{av}_{k+1}^\alpha(G). \qquad (5.2.3)$$

∎

Corollary 5.2.5. *For any n-vertex graph G we have $\mathrm{av}^{\alpha}(K_n) \geq \mathrm{av}^{\alpha}(G)$, with equality only if $G = K_n$.*

Proof. By Theorem 5.2.4 and Lemma 5.2.2 we get

$$\mathrm{av}^{\alpha}(K_n) = \mathrm{av}^{\alpha}_{\lfloor n/2 \rfloor}(K_n) \geq \mathrm{av}^{\alpha}_{\mu(G)}(K_n) \geq \mathrm{av}^{\alpha}_{\mu(G)}(G) = \mathrm{av}^{\alpha}(G).$$

■

5.2.2 The case of trees

Let us first prove that the star minimizes the weighted average size of matchings among all n-vertex trees.

Theorem 5.2.6. *For every n-vertex tree $T \neq S_n$, $\mathrm{av}^{\alpha}(S_n) < \mathrm{av}^{\alpha}(T)$.*

Proof. Let us compute the average size of random matchings in a star.

$$\mathrm{av}^{\alpha}(S_n) = \frac{\alpha(n-1)}{1+\alpha(n-1)}.$$

For any other n-vertex tree, we have

$$\mathrm{av}^{\alpha}(T) = \frac{\alpha(n-1) + \sum_{i\geq 2} i\,\mathrm{m}(G,i)\alpha^i}{1+\alpha(n-1)+\sum_{i\geq 2}\mathrm{m}(G,i)\alpha^i},$$

where $\sum_{i\geq 2} i\,\mathrm{m}(G,i)\alpha^i \geq \sum_{i\geq 2}\mathrm{m}(G,i)\alpha^i > 0$.

Now we obtain:

$$\begin{aligned}
&\mathrm{av}^{\alpha}(T) - \mathrm{av}^{\alpha}(S_n)\\
&= \frac{\alpha(n-1) + \sum_{i\geq 2} i\,\mathrm{m}(G,i)\alpha^i}{1+\alpha(n-1)+\sum_{i\geq 2}\mathrm{m}(G,i)\alpha^i} - \frac{\alpha(n-1)}{1+\alpha(n-1)}\\
&= \frac{(1+\alpha(n-1))\left(\sum_{i\geq 2} i\,\mathrm{m}(G,i)\alpha^i\right) - \alpha(n-1)\left(\sum_{i\geq 2}\mathrm{m}(G,i)\alpha^i\right)}{\left(1+\alpha(n-1)+\sum_{i\geq 2}\mathrm{m}(G,i)\alpha^i\right)(1+\alpha(n-1))}\\
&= \frac{\sum_{i\geq 2} i\,\mathrm{m}(G,i)\alpha^i + \alpha(n-1)\left(\sum_{i\geq 2} i\,\mathrm{m}(G,i)\alpha^i - \sum_{i\geq 2}\mathrm{m}(G,i)\alpha^i\right)}{\left(1+\alpha(n-1)+\sum_{i\geq 2}\mathrm{m}(G,i)\alpha^i\right)(1+\alpha(n-1))}\\
&> 0.
\end{aligned}$$

■

For the problem of maximization, as in the case of the weighted average size of independent sets, let us first consider the situation where $\alpha \in [0,1]$. The line graph of the n-vertex path P_n is the $(n-1)$-vertex path P_{n-1}. This implies that the matchings of P_n can be identified with the independent sets of P_{n-1}. Thus, the weighted average size of matchings of P_n ($\mathrm{av}^\alpha(P_n)$) is the same as the average size of the independent sets of P_{n-1} ($\mathrm{avi}^\alpha(P_{n-1})$). Using the same approach as for the weighted independent sets, we obtain the following lemma.

Lemma 5.2.7. *The weighted average size of matchings of the n-vertex path P_n is*

$$\begin{aligned}\mathrm{av}^\alpha(P_n) &= \mathrm{avi}^\alpha(P_{n-1})\\ &= \frac{1+4\alpha-\sqrt{1+4\alpha}}{2(1+4\alpha)}n + \frac{1-\sqrt{1+4\alpha}}{2(1+4\alpha)} - \frac{(n+1)\alpha^{n+1}}{\sqrt{1+4\alpha}((-\phi_\alpha^2)^{n+1}-\alpha^{n+1})},\end{aligned} \tag{5.2.4}$$

where $\phi_\alpha = \frac{\sqrt{1+4\alpha}+1}{2}$. In particular,

(a) $\displaystyle\lim_{n\to\infty} \mathrm{av}^\alpha(P_n) - \frac{1+4\alpha-\sqrt{1+4\alpha}}{2(1+4\alpha)}n = \frac{1-\sqrt{1+4\alpha}}{2(1+4\alpha)}$,

(b) $\mathrm{av}^\alpha(P_n) \le \dfrac{1+4\alpha-\sqrt{1+4\alpha}}{2(1+4\alpha)}n + \dfrac{1}{\sqrt{1+4\alpha}} - \dfrac{1}{\alpha+1}$, *with equality only for $n = 2$. For all positive integers $n \neq 2$, we even have* $\mathrm{av}^\alpha(P_n) \le \dfrac{1+4\alpha-\sqrt{1+4\alpha}}{2(1+4\alpha)}n + \dfrac{2}{\sqrt{1+4\alpha}} - \dfrac{3\alpha+2}{\alpha^2+3\alpha+1}$.

For ease of notation, we set $a = \frac{1+4\alpha-\sqrt{1+4\alpha}}{2(1+4\alpha)}$ and $c_n(\alpha) = \mathrm{av}^\alpha(P_n) - an$. Let us give values of $c_n(\alpha)$ for small n:

$$\begin{aligned}
c_1(\alpha) &= -\frac{1}{2} + \frac{1}{2\sqrt{1+4\alpha}}\\
c_2(\alpha) &= -\frac{1}{\alpha+1} + \frac{1}{\sqrt{1+4\alpha}}\\
c_3(\alpha) &= -\frac{2\alpha+3}{2(2\alpha+1)} + \frac{3}{2\sqrt{1+4\alpha}}\\
c_4(\alpha) &= -\frac{3\alpha+2}{\alpha^2+3\alpha+1} + \frac{2}{\sqrt{1+4\alpha}}\\
c_5(\alpha) &= -\frac{3\alpha^2+12\alpha+5}{2(3\alpha^2+4\alpha+1)} + \frac{5}{2\sqrt{1+4\alpha}}.
\end{aligned}$$

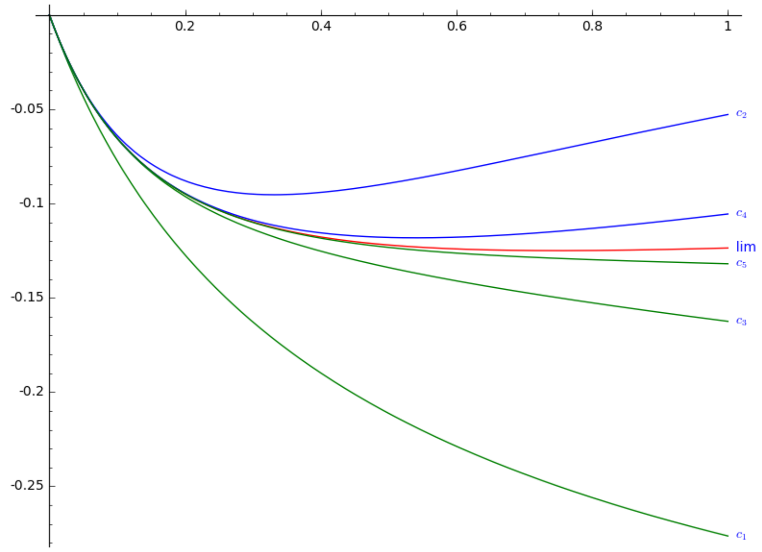


Figure 5.1: Values of $c_n(\alpha)$ for $n = 1, \dots, 5$ and the limit $\frac{1-\sqrt{1+4\alpha}}{2(1+4\alpha)}$.

Before we prove our main result, we require one more lemma:

Lemma 5.2.8. *For every tree T and every vertex v of T, we have*

$$\frac{1}{1+\alpha d(v)} \leq \frac{\mathrm{M}^\alpha(T-v)}{\mathrm{M}^\alpha(T)} < 1.$$

Proof. Note first that $\mathrm{M}^\alpha(T) = \mathrm{M}^\alpha(T-v) + \alpha \sum_{uv \in E(T)} M(T-v-u)$. Since $T-v-u$ is a subgraph of $T-v$, we have $\mathrm{M}^\alpha(T-v-u) \leq \mathrm{M}^\alpha(T-v)$, hence $(1+\alpha d(v))\,\mathrm{M}^\alpha(T-v) \geq \mathrm{M}^\alpha(T)$, which proves the first inequality. The second inequality simply follows from the fact that $T-v$ is a proper subgraph of T. ■

Theorem 5.2.9. *For every $\alpha \in (0,1]$ and every tree T of order n that is not a path, we have the inequality $\mathrm{av}^\alpha(T) \leq an + c_5(\alpha)$. Consequently, the path maximises the value of $\mathrm{av}^\alpha(T)$ among all trees of order n.*

Proof. We prove the inequality by induction on n. For $n \leq 3$, there is nothing to prove since the only trees with three or fewer vertices are paths. Thus assume now that $n \geq 4$, and consider a vertex v of the tree T whose degree is at least 3 (which must exist if T is not a path). Denote the neighbours of v by $v_1, v_2, \dots, v_k$ and the components of $T - v$ by $T_1, T_2, \dots, T_k$ (in such a way that v_j is contained in T_j). Let e be the edge between v and v_k, and $T' = T - T_k$ be the tree obtained by removing T_k from T. We have

$$\begin{aligned}
\mathrm{av}^{\alpha}(T) &= \frac{\mathrm{S}^{\alpha}(T)}{\mathrm{M}^{\alpha}(T)} \\
&= \frac{\mathrm{S}^{\alpha}(T-e) + \alpha(\mathrm{S}^{\alpha}(T-v-v_k) + \mathrm{M}^{\alpha}(T-v-v_k))}{\mathrm{M}^{\alpha}(T)} \\
&= \frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)} \cdot \frac{\mathrm{S}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T-e)} + \frac{\alpha\,\mathrm{M}^{\alpha}(T-v-v_k)}{\mathrm{M}^{\alpha}(T)} \cdot \Big(1 + \frac{\mathrm{S}^{\alpha}(T-v-v_k)}{\mathrm{M}^{\alpha}(T-v-v_k)}\Big) \\
&= \frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)}\,\mathrm{av}^{\alpha}(T-e) + \frac{\mathrm{M}^{\alpha}(T) - \mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)}(1 + \mathrm{av}^{\alpha}(T-v-v_k)) \\
&= \frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)}(\mathrm{av}^{\alpha}(T') + \mathrm{av}^{\alpha}(T_k)) + \Big(1 - \frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)}\Big) \\
&\Big(1 + \sum_{j=1}^{k-1} \mathrm{av}^{\alpha}(T_j) + \mathrm{av}^{\alpha}(T_k - v_k)\Big) \\
&= \frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)} A(\alpha) + \Big(1 - \frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)}\Big) B(\alpha).
\end{aligned}$$

Assume first that $k \geq 4$. By Lemma 5.2.7 and the induction hypothesis, we have $\mathrm{av}^{\alpha}(T_j) \leq a|T_j| + c_2(\alpha)$ for all j and $\mathrm{av}^{\alpha}(T') \leq a|T'| + c_5(\alpha)$. It follows that

$$A(\alpha) \leq a(|T'| + |T_k|) + c_5(\alpha) + c_2(\alpha) < a|T| + c_5(\alpha).$$

If $B(\alpha) \leq a|T| + c_5(\alpha)$, then we are done. Hence we can assume $A(\alpha) < a|T| + c_5(\alpha) \leq B(\alpha)$. This implies that $\mathrm{av}^{\alpha}(T)$ is now decreasing regarded as a function of $\frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)}$. So let us find an explicit formula for $\frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)}$. We observe that:

$$\frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)} = \frac{\mathrm{M}^{\alpha}(T')\,\mathrm{M}^{\alpha}(T_k)}{\mathrm{M}^{\alpha}(T')\,\mathrm{M}^{\alpha}(T_k) + \alpha\,\mathrm{M}^{\alpha}(T'-v)\,\mathrm{M}^{\alpha}(T_k - v_k)},$$

thus

$$\frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)} = \frac{1}{1 + \alpha \cdot \frac{\mathrm{M}^{\alpha}(T'-v)}{\mathrm{M}^{\alpha}(T')} \cdot \frac{\mathrm{M}^{\alpha}(T_k - v_k)}{\mathrm{M}^{\alpha}(T_k)}}. \tag{5.2.5}$$

Moreover,

$$\begin{aligned}
\frac{\mathrm{M}^{\alpha}(T'-v)}{\mathrm{M}^{\alpha}(T')} &= \frac{\prod_j^{k-1} \mathrm{M}^{\alpha}(T_j)}{\prod_j^{k-1} \mathrm{M}^{\alpha}(T_j) + \alpha \sum_j^{k-1} \frac{\prod_j^{k-1} \mathrm{M}^{\alpha}(T_j)}{\mathrm{M}^{\alpha}(T_j)} \cdot \mathrm{M}^{\alpha}(T_j - v_j)} \\
&= \frac{1}{1 + \alpha \sum_j^{k-1} \frac{\mathrm{M}^{\alpha}(T_j - v_j)}{\mathrm{M}^{\alpha}(T_j)}}. \qquad (5.2.6)
\end{aligned}$$

Two cases can be considered:

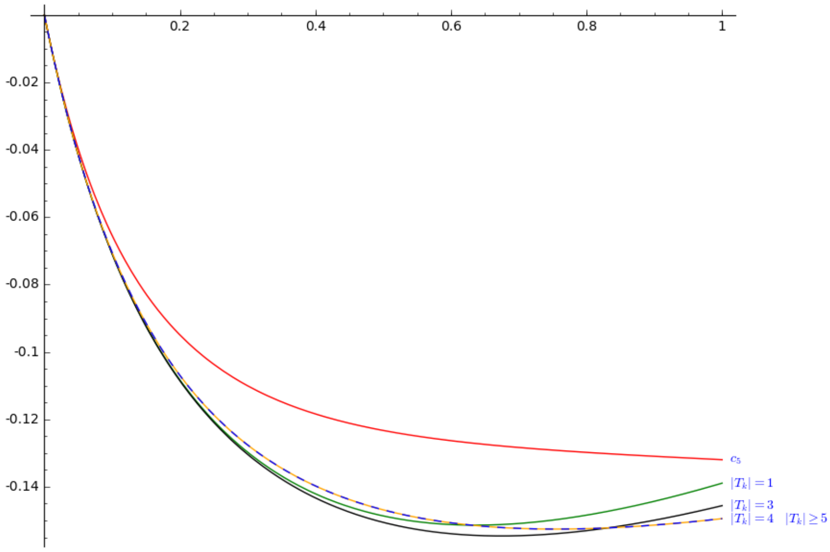


Figure 5.2: Case 1.

Case 1: None of the T_j's is P_2. By Lemma 5.1.10, $\frac{\mathrm{M}^\alpha(T'-v)}{\mathrm{M}^\alpha(T')} \leq 1$, and plugging this estimate in Equation (5.2.5), we obtain

$$\frac{\mathrm{M}^\alpha(T-e)}{\mathrm{M}^\alpha(T)} \geq \frac{1}{1+\alpha\frac{\mathrm{M}^\alpha(T_k-v_k)}{\mathrm{M}^\alpha(T_k)}}. \tag{5.2.7}$$

Moreover, by Lemma 5.2.7 and the induction hypothesis we have

$$\begin{aligned}\sum_{j=1}^{k-1}\mathrm{av}^\alpha(T_j) &\leq \sum_{j=1}^{k-1}(a|T_j|+c_4(\alpha)) \leq a(|T'|-1)+(k-1)c_4(\alpha)\\ &\leq a|T'|+3c_4(\alpha)-a.\end{aligned}$$

Now let us consider subcases depending on the order of T_k. We may assume that $|T_k| = \min_{1\leq j\leq k}|T_j|$.

- If $|T_k| = 1$, then $\mathrm{av}^\alpha(T_k) = \mathrm{av}^\alpha(T_k - v_k) = a|T_k| - a$. It follows that

$$\begin{aligned}A(\alpha) &\leq a|T'|+c_5(\alpha)+a|T_k|-a = a|T|+c_5(\alpha)-a,\\ B(\alpha) &\leq 1+a|T'|+3c_4(\alpha)-a+a|T_k|-a\\ &= a|T|+1-2a+3c_4(\alpha).\end{aligned}$$

Since $\frac{\mathrm{M}^{\alpha}(T_k - v_k)}{\mathrm{M}^{\alpha}(T_k)} = 1$, Equation (5.2.7) gives us $\frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)} \geq \frac{1}{\alpha+1}$. Thus,

$$\begin{aligned}
\mathrm{av}^{\alpha}(T) &\leq \frac{1}{\alpha+1}\left(a|T| + c_5(\alpha) - a\right) + \frac{\alpha}{\alpha+1}\left(a|T| + 1 - 2a + 3c_4(\alpha)\right) \\
&= a|T| + \frac{1}{\alpha+1}\left(c_5(\alpha) + 3\alpha c_4(\alpha) + (1-2a)\alpha - a\right) \\
&\leq a|T| + c_5(\alpha).
\end{aligned}$$

- If $|T_k| = 3$, then $\mathrm{av}^{\alpha}(T_k) = a|T_k| + c_3(\alpha)$ and $\mathrm{av}^{\alpha}(T_k - v_k) \leq a|T_k| - a + c_2(\alpha)$. It follows that

$$\begin{aligned}
A(\alpha) &\leq a|T'| + c_5(\alpha) + a|T_k| + c_3(\alpha) = a|T| + c_5(\alpha) + c_3(\alpha), \\
B(\alpha) &\leq 1 + a|T'| + 3c_4(\alpha) - a + a|T_k| - a + c_2(\alpha) \\
&= a|T| + 1 - 2a + 3c_4(\alpha) + c_2(\alpha).
\end{aligned}$$

Moreover, $\frac{\mathrm{M}^{\alpha}(T_k - v_k)}{\mathrm{M}^{\alpha}(T_k)} \leq \frac{\alpha+1}{2\alpha+1}$, so by Equation (5.2.7) $\frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)} \geq \frac{2\alpha+1}{\alpha^2+3\alpha+1}$. We obtain

$$\begin{aligned}
\mathrm{av}^{\alpha}(T) \leq{}& \frac{2\alpha+1}{\alpha^2+3\alpha+1}\left(a|T| + c_5(\alpha) + c_3(\alpha)\right) \\
&+ \frac{\alpha(\alpha+1)}{\alpha^2+3\alpha+1}\left(a|T| + 1 - 2a + 3c_4(\alpha) + c_2(\alpha)\right) \\
={}& a|T| + \frac{1}{\alpha^2+3\alpha+1}\big((2\alpha+1)(c_5(\alpha) + c_3(\alpha)) \\
&+ \alpha(\alpha+1)(3c_4(\alpha) + c_2(\alpha) + 1 - 2a)\big) \\
\leq{}& a|T| + c_5(\alpha).
\end{aligned}$$

- If $|T_k| = 4$, then $\mathrm{av}^{\alpha}(T_k) \leq a|T_k| + c_4(\alpha)$, and $\mathrm{av}^{\alpha}(T_k - v_k) \leq a|T_k| - a + c_3(\alpha)$. It follows that

$$\begin{aligned}
A(\alpha) &\leq a|T'| + c_5(\alpha) + a|T_k| + c_4(\alpha) = a|T| + c_5(\alpha) + c_4(\alpha), \\
B(\alpha) &\leq 1 + a|T'| + 3c_4(\alpha) - a + a|T_k| - a + c_3(\alpha) \\
&= a|T| + 1 - 2a + 3c_4(\alpha) + c_3(\alpha).
\end{aligned}$$

Moreover, $\frac{\mathrm{M}^\alpha(T_k - v_k)}{\mathrm{M}^\alpha(T_k)} \leq \frac{2\alpha+1}{3\alpha+1}$, so using Equation (5.2.7) again, we get $\frac{\mathrm{M}^\alpha(T-e)}{\mathrm{M}^\alpha(T)} \geq \frac{3\alpha+1}{2\alpha^2+4\alpha+1}$. Hence

$$\begin{aligned}
\mathrm{av}^\alpha(T) &\leq \frac{3\alpha+1}{2\alpha^2+4\alpha+1}\left(a|T| + c_5(\alpha) + c_4(\alpha)\right) \\
&\quad + \frac{\alpha(2\alpha+1)}{2\alpha^2+4\alpha+1}\left(a|T| + 1 - 2a + 3c_4(\alpha) + c_3(\alpha)\right) \\
&= a|T| + \frac{1}{2\alpha^2+4\alpha+1}((3\alpha+1)(c_5(\alpha)+c_4(\alpha)) \\
&\quad + \alpha(2\alpha+1)(3c_4(\alpha) + c_3(\alpha) + 1 - 2a)) \\
&\leq a|T| + c_5(\alpha).
\end{aligned}$$

- If $|T_k| \geq 5$, then $\mathrm{av}^\alpha(T_j) \leq a|T_j| + c_6(\alpha)$ for all j, and $\mathrm{av}^\alpha(T_k - v_k) \leq a|T_k| - a + c_4(\alpha)$. It follows that

$$\begin{aligned}
A(\alpha) &\leq a|T| + c_5(\alpha) + c_6(\alpha), \\
B(\alpha) &\leq 1 + a|T'| + 3c_6(\alpha) - a + a|T_k| - a + c_4(\alpha) \\
&= a|T| + 1 - 2a + 3c_6(\alpha) + c_4(\alpha).
\end{aligned}$$

Since $\frac{\mathrm{M}^\alpha(T_k - v_k)}{\mathrm{M}^\alpha(T_k)} \leq 1$, we have $\frac{\mathrm{M}^\alpha(T-e)}{\mathrm{M}^\alpha(T)} \geq \frac{1}{\alpha+1}$. Thus,

$$\begin{aligned}
\mathrm{av}^\alpha(T) &\leq \frac{1}{\alpha+1}\left(a|T| + c_5(\alpha) + c_6(\alpha)\right) \\
&\quad + \frac{\alpha}{\alpha+1}\left(a|T| + 1 - 2a + 3c_6(\alpha) + c_4(\alpha)\right) \\
&= a|T| + \frac{1}{\alpha+1}\left(c_5(\alpha) + c_6(\alpha) + \alpha(3c_6(\alpha) + c_4(\alpha) + 1 - 2a)\right) \\
&\leq a|T| + c_5(\alpha).
\end{aligned}$$

Case 2: One of the T_j's is P_2. We can assume without loss of generality that $T_k = P_2$. Let us observe two subcases depending on the number of P_2's among the T_j's.

- At least one of the T_j's is different from P_2. By Lemma 5.2.7 and the induction hypothesis

$$\begin{aligned}
A(\alpha) &\leq a|T| + c_5(\alpha) + c_2(\alpha), \\
B(\alpha) &\leq 1 + a(|T'| - 1) + 2c_2(\alpha) + c_4(\alpha) + a|T_k| - 2a \\
&= a|T| + 1 - 3a + 2c_2(\alpha) + c_4(\alpha).
\end{aligned}$$

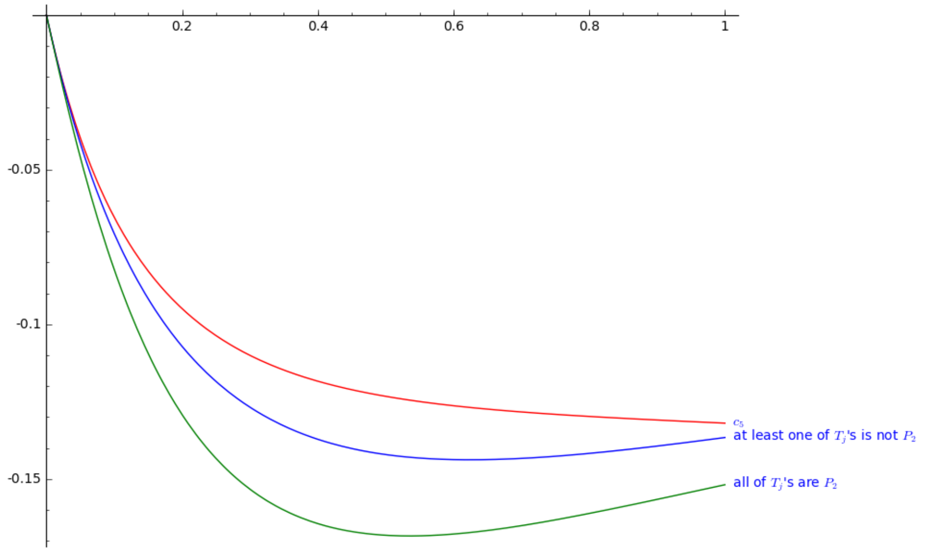


Figure 5.3: Case 2.

By Lemma 5.2.8, $\frac{\mathrm{M}^{\alpha}(T'-v)}{\mathrm{M}^{\alpha}(T')} \leq 1$, moreover $\frac{\mathrm{M}^{\alpha}(T_k-v_k)}{\mathrm{M}^{\alpha}(T_k)} = \frac{1}{\alpha+1}$. Using those values in Equation (5.2.5), we obtain $\frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)} \geq \frac{\alpha+1}{2\alpha+1}$. Thus,

$$
\begin{aligned}
\mathrm{av}^{\alpha}(T) \leq{} & \frac{\alpha+1}{2\alpha+1}\left(a|T| + c_5(\alpha) + c_2(\alpha)\right) \\
& + \frac{\alpha}{2\alpha+1}\left(a|T| + 1 - 3a + 2c_2(\alpha) + c_4(\alpha)\right) \\
={} & a|T| + \frac{\alpha+1}{2\alpha+1}\left(c_5(\alpha) + c_2(\alpha)\right) \\
& + \frac{\alpha}{2\alpha+1}\left(1 - 3a + 2c_2(\alpha)) + c_4(\alpha)\right) \\
={} & a|T| + \frac{1}{2\alpha+1}\Big((\alpha+1)(c_5(\alpha) + c_2(\alpha)) \\
& + \alpha(1 - 3a + 2c_2(\alpha) + c_4(\alpha))\Big) \\
\leq{} & a|T| + c_5(\alpha).
\end{aligned}
$$

- if all of the T_j's are equal to P_2, then by Lemma 5.2.7 and the induction hypothesis

$$
\begin{aligned}
A(\alpha) &\leq a|T| + c_5(\alpha) + c_2(\alpha), \\
B(\alpha) &\leq 1 + a(|T'| - 1) + 3c_2(\alpha) + a|T_k| - 2a \\
&= a|T| + 1 - 3a + 3c_2(\alpha).
\end{aligned}
$$

Now, from Equation (5.2.6), we have

$$\begin{aligned}\frac{\mathrm{M}^{\alpha}(T'-v)}{\mathrm{M}^{\alpha}(T')} &= \frac{1}{1+\alpha\sum_j^{k-1}\frac{\mathrm{M}^{\alpha}(T_j-v_j)}{\mathrm{M}^{\alpha}(T_j)}} \\ &= \frac{1}{1+(k-1)\frac{\alpha}{\alpha+1}} \le \frac{1}{1+3\frac{\alpha}{\alpha+1}} = \frac{\alpha+1}{4\alpha+1}.\end{aligned}$$

Plugging this estimate and the fact that $\frac{\mathrm{M}^{\alpha}(T_k-v_k)}{\mathrm{M}^{\alpha}(T_k)} = \frac{1}{\alpha+1}$ into Equation (5.2.5), we have

$$\frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)} \ge \frac{1}{1+\alpha\frac{\alpha+1}{4\alpha+1}\frac{1}{\alpha+1}} = \frac{4\alpha+1}{5\alpha+1}.$$

Therefore,

$$\begin{aligned}&\mathrm{av}^{\alpha}(T) \\ &\le \frac{4\alpha+1}{5\alpha+1}\left(a|T|+c_5(\alpha)+c_2(\alpha)\right)+\frac{\alpha}{5\alpha+1}\left(a|T|+1-3a+3c_2(\alpha)\right) \\ &= a|T|+\frac{1}{5\alpha+1}((4\alpha+1)(c_5(\alpha)+c_2(\alpha))+\alpha(1-3a+3c_2(\alpha))) \\ &\le a|T|+c_5(\alpha).\end{aligned}$$

This completes the case that $k \ge 4$, so we are left with the case that $k=3$. We return to the representation

$$\begin{aligned}\mathrm{av}^{\alpha}(T) &= \frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)}(\mathrm{av}^{\alpha}(T')+\mathrm{av}^{\alpha}(T_k)) \\ &\quad+\left(1-\frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)}\right)\left(1+\sum_{j=1}^{k-1}\mathrm{av}^{\alpha}(T_j)+\mathrm{av}^{\alpha}(T_k-v_k)\right).\end{aligned} \tag{5.2.8}$$

Using Equation (5.2.6) and Equation (5.2.5), we obtain

$$\frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)} = \frac{1}{1+\frac{\alpha}{1+\alpha\sum_j^{k-1}\frac{\mathrm{M}^{\alpha}(T_j-v_j)}{\mathrm{M}^{\alpha}(T_j)}}\cdot\frac{\mathrm{M}^{\alpha}(T_k-v_k)}{\mathrm{M}^{\alpha}(T_k)}}. \tag{5.2.9}$$

Now, let us distinguish different cases depending on how many of the branches T_j have one, two, three, four and five or more vertices respectively. This gives us a total of 35 cases corresponding to the solutions of

$$x_1+x_2+x_3+x_4+x_5 = 3.$$

Here, x_1, x_2, x_3, x_4 stand for the number of T_j's with one, two, three, four vertices respectively, and x_5 is the number of T_j's with five or more vertices. In each of the cases, we use the following explicit values and estimates:

$$\mathrm{av}^\alpha(T_j) \begin{cases} = a|T_j| - a & |T_j| = 1, \\ = a|T_j| + c_2(\alpha) & |T_j| = 2, \\ = a|T_j| + c_3(\alpha) & |T_j| = 3, \\ \leq a|T_j| + c_4(\alpha) & |T_j| = 4, \\ \leq a|T_j| + c_6(\alpha) & \text{otherwise}, \end{cases}$$

$$\mathrm{av}^\alpha(T_j - v_j) \begin{cases} = a|T_j| - a & |T_j| = 1, \\ = a|T_j| - 2a & |T_j| = 2, \\ \leq a|T_j| + c_2(\alpha) - a & |T_j| = 3, \\ \leq a|T_j| + c_3(\alpha) - a & |T_j| = 4, \\ \leq a|T_j| + c_4(\alpha) - a & \text{otherwise}. \end{cases}$$

Using Lemma 5.2.8, we have

$$\frac{\mathrm{M}^\alpha(T_j - v_j)}{\mathrm{M}^\alpha(T_j)} \begin{cases} = 1 & |T_j| = 1, \\ = \frac{1}{\alpha+1} & |T_j| = 2, \\ \in [\frac{1}{2\alpha+1}, \frac{\alpha+1}{2\alpha+1}] & |T_j| = 3, \\ \in [\frac{\alpha+1}{\alpha^2+3\alpha+1}, \frac{2\alpha+1}{3\alpha+1}] & |T_j| = 4, \\ \in [\frac{3\alpha+1}{5\alpha^2+5\alpha+1}, \frac{2\alpha+1}{3\alpha+1}] & \text{otherwise}. \end{cases}$$

Let us consider the last case for example. We can assume that the outdgree of v_j, which is its degree when removing v, is at most 2, since otherwise $d(v_j) \geq 4$ and we can go back to the previous cases. Using Equation (5.2.6), we have

$$\frac{\mathrm{M}^\alpha(T_j - v_j)}{\mathrm{M}^\alpha(T_j)} = \frac{1}{1 + \alpha\left(\frac{M^\alpha(T_{j_1} - v_{j_1})}{M^\alpha(T_{j_1})} + \frac{M^\alpha(T_{j_2} - v_{j_2})}{M^\alpha(T_{j_2})}\right)}. \tag{5.2.10}$$

Now, by Lemma 5.2.8, we have $\frac{\mathrm{M}^\alpha(T_{j_i} - v_{j_i})}{\mathrm{M}^\alpha(T_{j_i})} \geq \frac{1}{2\alpha+1}$. Hence,

$$\frac{\mathrm{M}^\alpha(T_j - v_j)}{\mathrm{M}^\alpha(T_j)} \leq \frac{1}{1 + \alpha\frac{M^\alpha(T_{j_1} - v_{j_1})}{M^\alpha(T_{j_1})}} \leq \frac{1}{1 + \frac{\alpha}{2\alpha+1}} = \frac{2\alpha+1}{3\alpha+1}. \tag{5.2.11}$$

For the lower bound, by Lemma 5.2.8, we have $\frac{\mathrm{M}^{\alpha}(T_{ji}-v_{ji})}{\mathrm{M}^{\alpha}(T_{ji})} \leq 1$. Note that we cannot put this estimate in for both the branches of T_j, since then the order of T_j would be equal to 3 while we need $|T_j| \geq 5$. So, we plug the bound (5.2.11) into Equation (5.2.10) for one of the branches and get

$$\begin{aligned} \frac{\mathrm{M}^{\alpha}(T_j - v_j)}{\mathrm{M}^{\alpha}(T_j)} &\geq \frac{1}{1+\alpha\left(\frac{M^{\alpha}(T_{j1}-v_{j1})}{M^{\alpha}(T_{j1})}+1\right)} \\ &\geq \frac{1}{1+\alpha\left(1+\frac{2\alpha+1}{3\alpha+1}\right)} = \frac{3\alpha+1}{5\alpha^2+5\alpha+1}. \end{aligned} \tag{5.2.12}$$

We plug these estimates into (5.2.8) and also use the identity (5.2.9). Furthermore, $\mathrm{av}^{\alpha}(T') + \mathrm{av}^{\alpha}(T_k) \leq a|T| + c_2(\alpha) + c_4(\alpha) < a|T| + c_5(\alpha)$. As before, if $1 + \sum_j^{k-1} \mathrm{av}^{\alpha}(T_j) + \mathrm{av}^{\alpha}(T_j - v_j) \leq a|T| + c_5(\alpha)$, then we are done. So we may assume $\mathrm{av}^{\alpha}(T') + \mathrm{av}^{\alpha}(T_k) < a|T| + c_5(\alpha) \leq 1 + \sum_j^{k-1} \mathrm{av}^{\alpha}(T_j) + \mathrm{av}^{\alpha}(T_j - v_j)$. Hence the expression (5.2.8) is linear and decreasing in $\frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)}$, its maximum is attained for the smallest possible value of $\frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)}$. Moreover, by the induction hypothesis $\mathrm{av}^{\alpha}(T') \leq \mathrm{av}^{\alpha}(P_{|T'|})$. This gives us an upper bound for $\mathrm{av}^{\alpha}(T)$ in each of the aforementioned 35 cases, which can all be checked with a computer. As an example, let us consider the case which gives us the worst estimate: it is obtained for $x_1 = x_3 = x_4 = x_5 = 0$ and $x_2 = 3$. Let T_i be trees with two vertices for all i. We have

$$\mathrm{av}^{\alpha}(T_1) = a|T_1| + c_2(\alpha),\ \mathrm{av}^{\alpha}(T') \leq a|T'| + c_5(\alpha)$$

and

$$\mathrm{av}^{\alpha}(T_1 - v_1) = a|T_1| - 2a,\ \mathrm{av}^{\alpha}(T_2) = a|T_2| + c_2(\alpha),\ \mathrm{av}^{\alpha}(T_3) \leq a|T_3| + c_2(\alpha)$$

as well as

$$\frac{\mathrm{M}^{\alpha}(T-e)}{\mathrm{M}^{\alpha}(T)} = \frac{1}{1+\alpha\cdot\frac{1}{\alpha+1}\cdot\frac{1}{1+\frac{2\alpha}{\alpha+1}}} = \frac{3\alpha+1}{4\alpha+1}.$$

Thus

$$\begin{aligned} \mathrm{av}^{\alpha}(T_1) + \mathrm{av}^{\alpha}(T') &\leq a(|T_1| + |T'|) + c_2(\alpha) + c_5(\alpha) \\ &= a|T| + c_2(\alpha) + c_5(\alpha), \end{aligned}$$

and likewise

$$\begin{aligned}\mathrm{av}^{\alpha}(T_1 - v_1) + \mathrm{av}^{\alpha}(T_2) + \mathrm{av}^{\alpha}(T_3) &\leq a(|T_1| + |T_2| + |T_3|) + 2c_2(\alpha) - 2a \\ &\leq a|T| + 2c_2(\alpha) - 3a.\end{aligned}$$

Putting everything together, we obtain

$$\begin{aligned}\mathrm{av}^{\alpha}(T) &= \frac{3\alpha+1}{4\alpha+1}\Big(a|T| + c_2(\alpha) + c_5(\alpha)\Big) \\ &\quad + \frac{\alpha}{4\alpha+1}\Big(1 + a|T| + 2c_2(\alpha) - 3a\Big) \\ &= a|T| + \frac{1}{4\alpha+1}\left((3\alpha+1)(c_2(\alpha) + c_5(\alpha) + \alpha(1 + 2c_2(\alpha) - 3a))\right) \\ &< a|T| + c_5(\alpha).\end{aligned}$$

The worst case is colored in green in Figure 5.4.

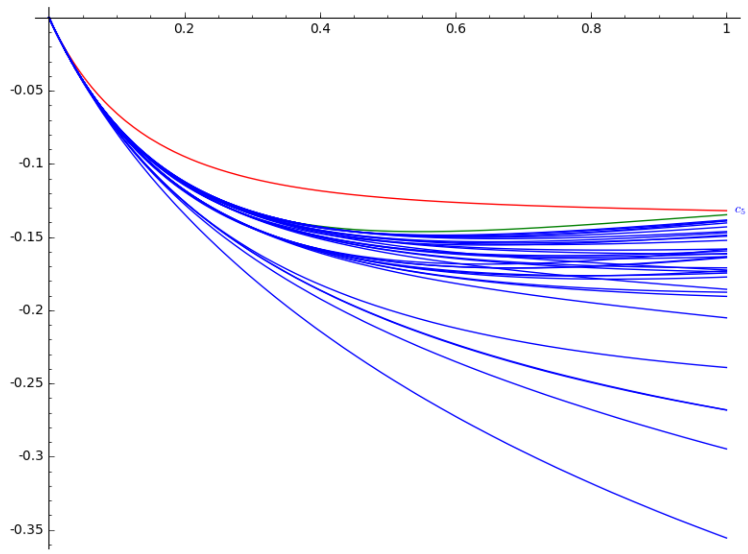


Figure 5.4: The 35 cases when $k = 3$.

However, we already know from Lemma 5.2.7 that

$$\mathrm{av}^{\alpha}(P_n) \geq an + c_5(\alpha)$$

for $n > 3$. Thus $\mathrm{av}^{\alpha}(P_n) \geq an + c_5(\alpha) \geq \mathrm{av}^{\alpha}(T)$ for every tree T with n vertices other than P_n. This completes the proof. ■

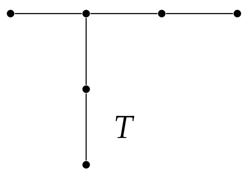
Analogously to the independent sets Theorems 5.2.6 and 5.2.9 give us the extremality of number of matchings:

Corollary 5.2.10. *For every n-vertex tree T,*

$$\mathrm{M}(S_n) \leq \mathrm{M}(T) \leq \mathrm{M}(P_n).$$

Proof. In fact $\int_0^1 \frac{\mathrm{av}^\alpha(T)}{\alpha} d\alpha = \log \mathrm{I}(G)$. Thus, the extremal trees for the weighted average size of matchings are also extremal for the number of matchings. ∎

For $\alpha > 1$, the path is not always the tree which maximizes the weighted average size of matchings. Let us consider trees of order 6. Let T be the following tree:



We have:

$$\mathrm{av}^\alpha(T) = \frac{3\alpha^3 + 10\alpha^2 + 5\alpha}{\alpha^3 + 5\alpha^2 + 5\alpha + 1},$$
$$\mathrm{av}^\alpha(P_7) = \frac{3\alpha^3 + 12\alpha^2 + 5\alpha}{\alpha^3 + 6\alpha^2 + 5\alpha + 1},$$

and $\mathrm{av}^3(T) \approx 2.11363 > \mathrm{av}^3(P_7) \approx 2.10309$.

Now, as for the case of independent sets, let us consider the case when α tends to infinity.

Let τ be the maximum size of matchings in T. Then

$$\begin{aligned}
\mathrm{M}^\alpha(T) &= \sum_{k\geq 0} \mathrm{m}(k,T)\alpha^k = 1 + \cdots + \mathrm{m}(\tau-1,T)\alpha^{\tau-1} + \mathrm{m}(\tau,T)\alpha^\tau, \\
\mathrm{S}^\alpha(T) &= \sum_{k\geq 0} k\,\mathrm{m}(k,T)\alpha^k \\
&= \mathrm{m}(1,T)\alpha + \cdots + (\tau-1)\,\mathrm{m}(\tau-1,T)\alpha^{\tau-1} + \tau\,\mathrm{m}(\tau,T)\alpha^\tau.
\end{aligned}$$

Thus,

$$\mathrm{av}^\alpha(T) = \frac{\tau\,\mathrm{m}(\tau,T)\alpha^\alpha + (\tau-1)\,\mathrm{m}(\tau-1,T)\alpha^{\tau-1} + \cdots + \mathrm{m}(1,T)\alpha}{\mathrm{m}(\tau,T)\alpha^\tau + \mathrm{m}(\tau-1,T)\alpha^{\tau-1} + \cdots + 1}. \tag{5.2.13}$$

When $\alpha \to \infty$, we get from Equation (5.2.13) that

$$\operatorname{av}^{\alpha}(T) = \frac{\tau\,\mathrm{m}(\tau,T) + (\tau-1)\,\mathrm{m}(\tau-1,T)\alpha^{-1} + \cdots + \mathrm{m}(1,T)\alpha^{1-\tau}}{\mathrm{m}(\tau,T) + \mathrm{m}(\tau-1,T)\alpha^{-1} + \cdots + \alpha^{-\tau}} \tag{5.2.14}$$

$$\to \tau.$$

Hence, for sufficiently large α, the tree that maximizes $\operatorname{av}^{\alpha}(T)$ must have the greatest possible matching number τ.

Furthermore, if we multiply both numerator and denominator by $\mathrm{m}(\tau,T) - \mathrm{m}(\tau-1,T)\alpha^{-1}$ in Equation (5.2.14), we obtain

$$\begin{aligned}\operatorname{av}^{\alpha}(T) &= \frac{\tau\,\mathrm{m}(\tau,T)^2 - \mathrm{m}(\tau,T)\,\mathrm{m}(\tau-1,T)\alpha^{-1} + \mathcal{O}(\alpha^{-2})}{\mathrm{m}(\tau,T)^2 + \mathcal{O}(\alpha^{-2})},\\ &= \tau - \frac{\mathrm{m}(\tau-1,T)}{\mathrm{m}(\tau,T)}\alpha^{-1} + \mathcal{O}(\alpha^{-2}).\end{aligned}$$

Hence, the “optimal" tree should also minimize $\frac{\mathrm{m}(\tau-1,T)}{\mathrm{m}(\tau,T)}$ for large enough α.

Proposition 5.2.11. *For large enough α, the tree that maximizes $\operatorname{av}^{\alpha}(T)$ has to have the greatest possible matching number τ and among all trees with this property, minimum $\frac{\mathrm{m}(\tau-1,T)}{\mathrm{m}(\tau,T)}$.*

We say that a tree maximizes the weighted average size of matchings at “infinity" if it maximizes $\operatorname{av}^{\alpha}(T)$ for sufficiently large α.

Theorem 5.2.12. *Among trees of order $n \leq 4$, the path P_n maximizes the average size of matchings at infinity.*

Proof.
- For $n \leq 3$, there is nothing to prove since the only tree of three or fewer vertices are paths.
- For $n = 4$, the trees of this order are the path P_4 and the star S_4. We already proved that S_4 is the one that minimizes the weighted average size of independent sets for any α.

∎

Conjecture 5.2.13. Among trees of order $n \geq 5$,

- if n is even, then the starlike tree $S(2,2,\ldots,2,1)$ (see Definition 2.3.6) maximizes the average size of matchings at infinity,
- otherwise the starlike tree $S(2,2,\ldots,2)$ maximizes the average size of matchings at infinity.

5.3 Relation with the matching energy

Let G be an n-vertex graph. The matching polynomial and the generating matching polynomial were defined in Chapter 1 as:

$$\varphi(G,x) = \sum_{k\geq 0} \mathrm{m}(G,k)(-1)^k x^{n-2k},$$
$$\mathrm{M}(G,x) = \sum_{k\geq 0} \mathrm{m}(G,k)x^k,$$

while the average size of matchings in G is

$$\mathrm{av}^{\alpha}(G) = \frac{\mathrm{M}'(G,1)}{\mathrm{M}(G,1)} = \frac{\sum_{k\geq 0} k\,\mathrm{m}(G,k)}{\sum_{k\geq 0}\mathrm{m}(G,k)},$$

where $\mathrm{M}'(G,x)$ is the first derivative of $\mathrm{M}(G,x)$ with respect to x.

Let $\mu_1, \mu_2, \ldots, \mu_n$ be the zeros of the matching polynomial $\varphi(G,x)$.Then, the matching energy [30] is defined as follows:

$$\mathrm{ME}(G) = \sum_{i=1}^{n} |\mu_i|.$$

We want to show a correspondence between the average size of matchings in G and the matching energy of G. Let us first relate φ and M.

$$\begin{aligned}\frac{\varphi(G,x)}{x^n} &= \sum_{k\geq 0} \mathrm{m}(G,k)(-1)^k x^{-2k}\\ &= \sum_{k\geq 0} \mathrm{m}(G,k)(-1)^k \left(\frac{1}{x^2}\right)^k\\ &= \mathrm{M}\left(G, -\frac{1}{x^2}\right).\end{aligned}$$

From this relation, we can write the derivative of φ in terms of M and its derivative.

$$\varphi'(G,x) = nx^{n-1}\,\mathrm{M}\left(G,-\frac{1}{x^2}\right) + 2x^{n-3}\,\mathrm{M}'\left(G,-\frac{1}{x^2}\right).$$

This gives us

$$\frac{\varphi'(G,x)}{\varphi(G,x)} = \frac{n}{x} + \frac{2}{x^3}\frac{\mathrm{M}'\left(G,-\frac{1}{x^2}\right)}{\mathrm{M}\left(G,-\frac{1}{x^2}\right)}. \tag{5.3.1}$$

Furthermore, we can rewrite φ and φ' as follows:

$$\varphi(G,x) = \prod_{i=1}^{n}(x-\mu_i),$$
$$\varphi'(G,x) = \sum_{j=1}^{n} \frac{\prod_{i=1}^{n}(x-\mu_i)}{x-\mu_j}.$$

Therefore,

$$\frac{\varphi'(G,x)}{\varphi(G,x)} = \sum_{j=1}^{n} \frac{1}{x-\mu_j}. \tag{5.3.2}$$

Now, we can establish a relation between the average size of matchings of G and the zeros of its matching polynomial.

Lemma 5.3.1. *Let G be an n-vertex graph and $\mu_1, \ldots, \mu_n$ be the zeros of the matching polynomial of G. Then,*

$$\operatorname{av}(G) = \frac{1}{2}\sum_{j=1}^{n} \frac{\mu_j^2}{\mu_j^2+1}.$$

Proof. Using (5.3.1) and (5.3.2), and plugging in $x = i$, we obtain

$$\sum_{j=1}^{n} \frac{1}{i-\mu_j} = \frac{n}{i} + \frac{2}{i^3}\frac{\mathrm{M}'(G,1)}{\mathrm{M}(G,1)}$$
$$\sum_{j=1}^{n} \frac{1}{i-\mu_j} + ni = 2i\operatorname{av}(G)$$
$$\sum_{j=1}^{n} \frac{1}{i-\mu_j} + i\sum_{j=1}^{n}\frac{i-\mu_j}{i-\mu_j} = 2i\operatorname{av}(G)$$
$$\sum_{j=1}^{n} \frac{\mu_j}{\mu_j-i} = 2\operatorname{av}(G). \tag{5.3.3}$$

Let us rearrange the left hand side of Equation (5.3.3). We have

$$\sum_{j=1}^{n} \frac{\mu_j}{\mu_j-i} = \sum_{j=1}^{n} \frac{\mu_j(\mu_j+i)}{(\mu_j-i)(\mu_j+i)} = \sum_{j=1}^{n} \frac{\mu_j^2+i\mu_j}{\mu_j^2+1}.$$

Identifying the two sides of the equation, we get the desired result. ∎

Having established this relation, we can now show a bound for the matching energy in terms of the average size of matchings.

Theorem 5.3.2. *Let G be a graph. Then,*

$$\mathrm{ME}(G) \geq 4\,\mathrm{av}(G).$$

Proof. Using Lemma 5.3.1 and the symmetry of the zeros of the matching polynomial, we have:

$$\mathrm{av}^{\alpha}(G) = \frac{1}{2}\sum_{j=1}^{n}\frac{\mu_j^2}{\mu_j^2+1} = \sum_{j|\mu_j>0}\frac{\mu_j^2}{\mu_j^2+1}.$$

Moreover, since for all j, $\frac{\mu_j}{\mu_j^2+1} \leq \frac{1}{2}$, we get

$$\mathrm{av}^{\alpha}(G) \leq \frac{1}{2}\sum_{j|\mu_j>0}\mu_j = \frac{1}{4}\mathrm{ME}(G).$$

∎

Remark 5.3.3. Note that for the case of trees, the matching polynomial coincides with the characteristic polynomial as in Proposition 2.4.12. So, we have a correspondence between the average size of matchings of a tree and the classical energy of a graph, which is the sum of the absolute values of the eingenvalues.

Now, let us consider a random matching where matchings of size k are chosen with probability proportional to α^k. The weighted average size of matchings in G is

$$\mathrm{av}^{\alpha}(G) = \frac{\sum_{k\geq 0} k\,\mathrm{m}(G,k)\alpha^k}{\sum_{k\geq 0}\mathrm{m}(G,k)\alpha^k} = \frac{\alpha\,\mathrm{M}'(G,\alpha)}{\mathrm{M}(G,\alpha)}.$$

Lemma 5.3.4. *Let G be an n-vertex graph and $\mu_1,\ldots,\mu_n$ be the zeros of the matching polynomial of G. Then,*

$$\mathrm{av}^{\alpha}(G) = \frac{1}{2}\sum_{j=1}^{n}\frac{\alpha\mu_j^2}{\alpha\mu_j^2+1}.$$

Proof. Using (5.3.1) and (5.3.2), and plugging in $x = i\alpha^{-\frac{1}{2}}$, we obtain

$$\sum_{j=1}^{n}\frac{1}{i\alpha^{-\frac{1}{2}}-\mu_j} = \frac{n}{i\alpha^{-\frac{1}{2}}} + \frac{2}{i^3\alpha^{-\frac{3}{2}}}\frac{\mathrm{M}'(G,\alpha)}{\mathrm{M}(G,\alpha)}$$

$$\sum_{j=1}^{n}\frac{1}{i\alpha^{-\frac{1}{2}}-\mu_j} = -ni\alpha^{\frac{1}{2}} + 2i\alpha^{\frac{1}{2}}\alpha\frac{\mathrm{M}'(G,\alpha)}{\mathrm{M}(G,\alpha)}$$

$$\begin{aligned} \sum_{j=1}^{n} \frac{1}{i\alpha^{-\frac{1}{2}} - \mu_j} + ni\alpha^{\frac{1}{2}} &= 2i\alpha^{\frac{1}{2}} \operatorname{av}^{\alpha}(G) \\ \sum_{j=1}^{n} \frac{1}{i\alpha^{-\frac{1}{2}} - \mu_j} + i\alpha^{\frac{1}{2}} \sum_{j=1}^{n} \frac{i\alpha^{-\frac{1}{2}} - \mu_j}{i\alpha^{-\frac{1}{2}} - \mu_j} &= 2i\alpha^{\frac{1}{2}} \operatorname{av}^{\alpha}(G) \\ \sum_{j=1}^{n} \frac{\mu_j}{\mu_j - i\alpha^{-\frac{1}{2}}} &= 2 \operatorname{av}^{\alpha}(G). \end{aligned} \tag{5.3.4}$$

Let us rearrange the left hand side of Equation (5.3.4). We have

$$\sum_{j=1}^{n} \frac{\mu_j}{\mu_j - i\alpha^{-\frac{1}{2}}} = \sum_{j=1}^{n} \frac{\mu_j(\mu_j + i\alpha^{-\frac{1}{2}})}{(\mu_j - i\alpha^{-\frac{1}{2}})(\mu_j + i\alpha^{-\frac{1}{2}})} = \sum_{j=1}^{n} \frac{\mu_j^2 + i\alpha^{-\frac{1}{2}}\mu_j}{\mu_j^2 + \alpha^{-1}}.$$

Identifying the two sides of the equation, we get :

$$2 \operatorname{av}^{\alpha}(G) = \sum_{j=1}^{n} \frac{\mu_j^2}{\mu_j^2 + \alpha^{-1}} = \sum_{j=1}^{n} \frac{\alpha\mu_j^2}{\alpha\mu_j^2 + 1}.$$

■

Theorem 5.3.5. *Let G be a graph. Then,*

$$\mathrm{ME}(G) \geq \frac{4}{\sqrt{\alpha}} \operatorname{av}^{\alpha}(G).$$

Proof. Using Lemma 5.3.4 and the symmetry of the zeros of the matching polynomial, we have:

$$\operatorname{av}^{\alpha}(G) = \frac{1}{2} \sum_{j=1}^{n} \frac{\alpha\mu_j^2}{\alpha\mu_j^2 + 1} = \sum_{j|\mu_j>0} \frac{\alpha\mu_j^2}{\alpha\mu_j^2 + 1}.$$

Moreover, since for all j, $\frac{\sqrt{\alpha}\mu_j}{\alpha\mu_j^2+1} \leq \frac{1}{2}$, we get

$$\operatorname{av}^{\alpha}(G) \leq \frac{\sqrt{\alpha}}{2} \sum_{j|\mu_j>0} \mu_j = \frac{\sqrt{\alpha}}{4} \mathrm{ME}(G).$$

■

Chapter 6

Extremal trees with given degree sequence

Extremal problems on the set of trees with given degree sequence have been thoroughly studied for the last decades. Numerous indices were considered by means of quite diverse techniques. We can mention the Wiener index [53, 65, 66, 73], the Harary index [63], the number of subtrees [3, 74], the spectral radius [6], the spectral moments [2, 45], the Laplacian spectral radii [71] and the energy, the Hosoya-index and the Merrifield-Simmons index [1]. We refer to [72] for a survey on extremal problems for degree sequence. One interesting phenomenon is that the extremal trees regarding those distinct parameters have the same or very similar structures, they are either "greedy trees" or "alternatingly greedy trees". This chapter is concerned with a generalisation and unification of the results for trees with given degree sequence. Our approach is based on an exchange-extremal property, which is inspired by [1, 34].

6.1 Preliminaries

Let T be a rooted tree. The root of T is denoted by $\mathrm{r}(T)$. We write $T = [T_1, T_2, \ldots, T_k]$ if $T_1, T_2, \ldots, T_k$ are all the branches of $\mathrm{r}(T)$. Let v and w be two different leaves of a tree H. We denote by $[L_1, L_2, \ldots, L_k]vHw[R_1, R_2, \ldots, R_\ell]$ the tree obtained by merging the root of $[L_1, L_2, \ldots, L_k]$ with v and the root of $[R_1, R_2, \ldots, R_\ell]$ with w. See Figure 6.1.

Definition 6.1.1. A subgraph B of a tree T is called a *complete branch* of T if and only if there is an edge e such that B is one of the components of $T - e$. That is, T can be decomposed as in Figure 6.2, where B and $T - B$ are non-empty.

We denote by $rd(B)$ the degree of $\mathrm{r}(B)$ as a vertex of B.

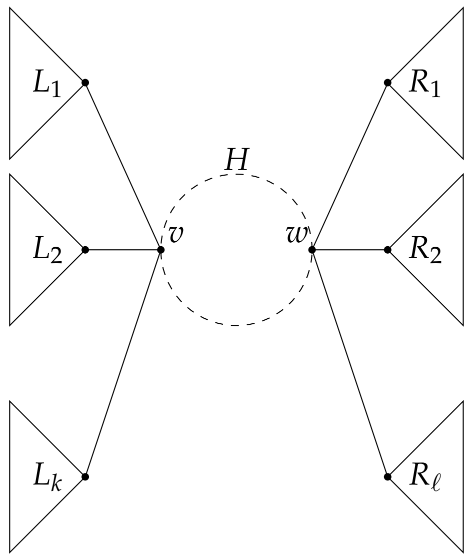


Figure 6.1: The tree $[L_1, L_2, \ldots, L_k]vHw[R_1, R_2, \ldots, R_\ell]$.

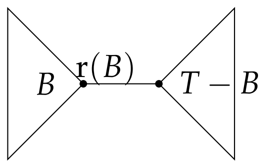


Figure 6.2: A complete branch.

Let $\rho(T)$ be a quantity associated to a rooted tree T, which satisfies the recursive relation

$$\rho([T_1, T_2, \ldots, T_k]) = f_\rho(\rho(T_1), \rho(T_2), \ldots, \rho(T_k)), \qquad (6.1.1)$$

for some symmetric function f_ρ, which means the value of f_ρ is independent at any permutation of the branches. We call f_ρ the recurrence rule for ρ.

Definition 6.1.2. We say that a tree T is ρ-exchange-extremal if whenever we have

$$T = [L_1, L_2, \dots, L_k]vHw[R_1, R_2, \dots, R_\ell],$$

for some H, then we have $k \geq \ell$ and

$$\min\{\rho(L_1), \rho(L_2), \dots, \rho(L_k)\} \geq \max\{\rho(R_1), \rho(R_2), \dots, \rho(R_\ell)\}$$

or $k \leq \ell$ and

$$\max\{\rho(L_1), \rho(L_2), \dots, \rho(L_k)\} \leq \min\{\rho(R_1), \rho(R_2), \dots, \rho(R_\ell)\}.$$

The following lemma is straightforward, but useful:

Lemma 6.1.3. *Let $T = [L_1, L_2, \dots, L_k]vHw[R_1, R_2, \dots, R_\ell]$ be a ρ-exchange extremal tree. If*

$$\min\{\rho(L_i) : 1 \leq i \leq k\} < \max\{\rho(R_i) : 1 \leq i \leq \ell\},$$

then we must have $k \leq \ell$ and

$$\max\{\rho(L_i) : 1 \leq i \leq k\} \leq \min\{\rho(R_i) : 1 \leq i \leq \ell\}.$$

6.2 Increasing recurrence rule f_ρ

In this section, we assume that, in addition to being symmetric, the function f_ρ is strictly increasing (strictly increasing in each single coordinate and strictly increasing under addition of further coordinates), and

$$\rho(\bullet) < \rho(B), \tag{6.2.1}$$

for all rooted trees B with $|V(B)| > 1$.

Definition 6.2.1. Given a degree sequence of a tree D, the greedy tree, denoted $G(D)$ is constructed by the following "greedy algorithm":

1. Label the vertex with the largest degree v (the root);
2. Label the neighbours of v as $v_1, v_2, \dots,$ and assign the largest degrees available to them such that $d(v_1) \geq d(v_2) \geq \cdots$;

3. Label the neighbours of v_1 (except v) as $v_{11}, v_{12}, \ldots$, and then do the same for $v_2, v_3, \ldots$;

4. Repeat (ii) and (iii) for all the newly labeled vertices. Always start with the neighbours of the labeled vertex with the largest degree whose neighbours are not labeled yet.

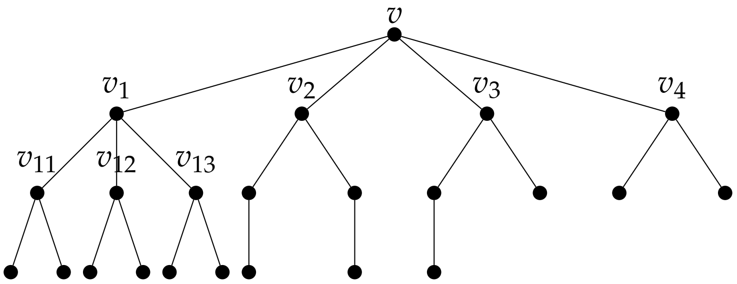


Figure 6.3: A greedy tree. (Only the first eight vertices are labelled).

Before we state and prove the main theorem of this section, let us first consider the special case where $\rho(T) = \rho_0(T) = |V(T)|$. If $T = [T_1, \ldots, T_k]$, we have

$$\rho_0(T) = 1 + \sum_{i=1}^{k} \rho_0(T_i).$$

The recurrence rule f_{ρ_0} is indeed symmetric and increasing with respect to any of its variables and under addition of further variables. Clearly $\rho_0(\bullet) = 1$ is minimum among all non-empty rooted trees. The following result is well-known:

Theorem 6.2.2 ([55]). *Given a degree sequence of a tree, if T is a ρ_0 exchange-extremal tree, then T is a greedy tree.*

Now, we are ready to prove the main theorem of this section.

Theorem 6.2.3. *Let ρ be an invariant of rooted trees that satisfies* (6.1.1) *and* (6.2.1) *for an increasing f_ρ. If a tree T is ρ-exchange-extremal, then T is a greedy tree.*

Proof. To prove this theorem, we only need to prove that for any complete branches A and B in T, $\rho(A) \leq \rho(B)$ if and only if $\rho_0(A) \leq \rho_0(B)$. Note that this also implies that $\rho(A) = \rho(B)$ if and only if $\rho_0(A) = \rho_0(B)$.

We reason by induction on $\max\{h(A), h(B)\}$. If $\max\{h(A), h(B)\} = 0$, then $h(A) = h(B) = 0$ and A and B are isomorphic rooted trees and the claim holds trivially. Assume that it holds whenever $\max\{h(A), h(B)\} \leq t$, for some $t \geq 0$. Now, consider the case where $\max\{h(A), h(B)\} = t + 1$. We assume there exist two complete branches A and B in T such that $\max\{h(A), h(B)\} = t+1$ and $\rho(A) \geq \rho(B)$. If $|V(B)| = 1$, then $\rho_0(A) \geq \rho_0(B) = \rho_0(\bullet)$ since f_{ρ_0} and f_ρ are increasing and $\rho_0(\bullet)$, $\rho(\bullet)$ are the respective minima. By the same arguments, if $|V(A)| = 1$, then $|V(B)| = 1$ since $\rho(A) \geq \rho(B)$. So, in both cases, there is nothing left to show. Now, we may assume $1 \notin \{|V(A)|, |V(B)|\}$. Let $A = [A_1, \ldots, A_k]$ and $B = [B_1, \ldots, B_\ell]$.

If $k \geq \ell$, by Definition 6.1.2, we have

$$\min\{\rho(A_i) : 1 \leq i \leq k\} \geq \max\{\rho(B_i) : 1 \leq i \leq \ell\},$$

then by the induction hypothesis, we have

$$\min\{\rho_0(A_i) : 1 \leq i \leq k\} \geq \max\{\rho_0(B_i) : 1 \leq i \leq \ell\}.$$

Thus $\rho_0(A) \geq \rho_0(B)$.

On the other hand, if $k \leq \ell$, by Definition 6.1.2 again, we have

$$\max\{\rho(A_i) : 1 \leq i \leq k\} \leq \min\{\rho(B_i) : 1 \leq i \leq \ell\},$$

then $\rho(A) \leq \rho(B)$ since f_ρ is increasing, so $\rho(A) = \rho(B)$. For this to hold, we must have $k = \ell$ and $\rho(A_1) = \cdots = \rho(A_k) = \rho(B_1) = \cdots = \rho(B_\ell)$. By the induction hypothesis, this implies $\rho_0(A_1) = \cdots = \rho_0(A_k) = \rho_0(B_1) = \cdots = \rho_0(B_\ell)$, so $\rho_0(A) = \rho_0(B)$.

Thus we have shown that $\rho(A) \geq \rho(B)$ implies $\rho_0(A) \geq \rho_0(B)$ and the converse is analogous.

∎

Remark 6.2.4. Note that f_ρ needs to be strictly increasing in each of its coordinates, otherwise we may have complete branches A and B such that $\rho(A) = \rho(B)$, but $\rho_0(A) \neq \rho_0(B)$.

6.3 Applications of Theorem 6.2.3

6.3.1 The Wiener index

The Wiener index of a tree T, introduced by Wiener [67], is one the oldest distance-based graph invariants and has been studied broadly in many papers. It is defined as the sum of all distances between all pairs of vertices:

$$W(T) = \sum_{u,v \in V(T)} d(u, v).$$

An alternative formulation of the Wiener index for trees is given as follows ([20]):

$$W(T) = \sum_{uv \in E(T)} |V(T_u)||V(T_v)|, \tag{6.3.1}$$

where T_u and T_v are respectively the components of T containing u and v after removing the edge uv.

Lemma 6.3.1. *Let T be a tree such that $W(T) \leq W(T')$ for every T' with the same degree sequence. For any complete branches $A = [A_1, \ldots, A_k]$ and $B = [B_1, \ldots, B_\ell]$ in T, we have either*

$k \geq \ell$ and

$$\min\{|V(A_1)|, \ldots, |V(A_k)|\} \geq \max\{|V(B_1)|, \ldots, |V(B_\ell)|\}$$

or $k \leq \ell$ and

$$\max\{|V(A_1)|, \ldots, |V(A_k)|\} \leq \min\{|V(B_1)|, \ldots, |V(B_\ell)|\}.$$

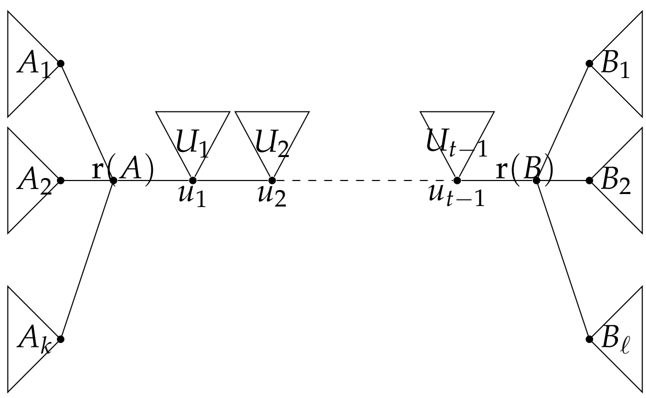


Figure 6.4: Decomposition of T in the proof of Lemma 6.3.1.

Proof. Let $\mathrm{r}(A) = u_0 u_1 \ldots u_t = \mathrm{r}(B)$ be the unique path between $\mathrm{r}(A)$ and $\mathrm{r}(B)$. To simplify notations, we put $\alpha = |V(A)|$ and $\beta = |V(B)|$.

For $0 < j < t$, let U_j be the subtree containing u_j when we remove all the edges of the path $P_T(\mathrm{r}(A), \mathrm{r}(B))$, and put $z_j = |V(U_j)|$. For convention, we will use $z_0 = z_t = 0$.

Put $p := p_0 + p_1 + \cdots + p_{t-1}$ with $p_i = z_0 + z_1 + \cdots + z_i$ and $q = q_0 + q_1 + \cdots + q_{t-1}$ with $q_i = z_t + z_{t-1} + \cdots + z_{t-i}$.

Using the expression for the Wiener index in (6.3.1), we have:

$$W(T) = \sum_{i=0}^{t-1} (\alpha + p_i)(q_{t-1-i} + \beta) + C_T.$$

Note that the contribution of edges in U_j, A and B does not depend on the permutation of A_i's and B_i's and thus is summarized in C_T.

$$\begin{aligned} W(T) &= \alpha q + \beta p + \alpha\beta + \sum_{i=0}^{t-1} p_i(q_{t-1-i}) + C_T && (6.3.2) \\ &= Wr(A_1, \ldots, A_k, B_1, \ldots, B_\ell) + \sum_{i=0}^{t-1} p_i q_{t-1-i} + C_T, && (6.3.3) \end{aligned}$$

The last two terms $\sum_{i=0}^{t} p_i(q_{t-i}) + C_T$ are invariants under any rearrangements of A_i's and B_i's. So the minimality of $W(T)$ can be deduced from $Wr(A_1, \ldots, A_k, B_1, \ldots, B_k)$. More precisely, if $W(T)$ is minimal, then for every permutation π of $\{A_1, \ldots A_k, B_1, \ldots, B_\ell\}$, we have

$$Wr(A_1, \ldots A_k, B_1, \ldots, B_\ell) \leq Wr(\pi(A_1), \ldots \pi(A_k), \pi(B_1), \ldots, \pi(B_\ell)).$$

Since the degree sequence is fixed, then the numbers k and ℓ are fixed. So, the product $\alpha\beta$ attains its minimum if and only if

$$k \leq \ell \text{ and } \max\{|V(A_j)| : 1 \leq j \leq k\} \leq \min\{|V(B_j)| : 1 \leq j \leq \ell\}$$

or

$$k \geq \ell \text{ and } \min\{|V(A_j)| : 1 \leq j \leq k\} \geq \max\{|V(B_j)| : 1 \leq j \leq \ell\}.$$

Next, the sum $\alpha q + \beta p$ is minimized if $p \leq q$, $k \geq \ell$ and,

$$\min\{|V(A_j)| : 1 \leq j \leq k\} \geq \max\{|V(B_j)|, x) : 1 \leq j \leq \ell\}$$

or $p \geq q$, $k \leq \ell$ and,

$$\max\{|V(A_j)| : 1 \leq j \leq k\} \leq \min\{|V(B_j) : 1 \leq j \leq \ell\}.$$

This concludes the proof of the lemma.

■

In any case, we find that the tree that minimizes the Wiener index must be ρ_0-exchange-extremal. Thus, we have

Theorem 6.3.2 ([73]). *The greedy tree minimizes the Wiener index among all trees with the same degree sequence.*

6.3.2 The terminal Wiener index

Let $\mathrm{Le}(T)$ be the set of leaves of a tree T. The terminal Wiener index of T ([55]) is the sum of all the distances between all pairs of leaves, more formally:

$$TW(T) = \sum_{u,v \in \mathrm{Le}(T)} d(u,v). \tag{6.3.4}$$

Analogously to the Wiener index, we may rewrite the terminal Wiener index as follows:

$$TW(T) = \sum_{uv \in E(T)} |\,\mathrm{Le}(T_u)||\,\mathrm{Le}(T_v)|, \tag{6.3.5}$$

where T_u and T_v are respectively the components of T containing u and v after removing the edge uv.

Lemma 6.3.3 ([55]). *Let T be a tree such that $TW(T) \leq TW(T')$ for every T' with the same degree sequence. For any complete branches $A = [A_1, \ldots, A_k]$ and $B = [B_1, \ldots, B_\ell]$ in T, we have either*

$k \geq \ell$ and

$$\min\{|\,\mathrm{Le}(A_1)|, \ldots, |\,\mathrm{Le}(A_k)|\} \geq \max\{|\,\mathrm{Le}(B_1)|, \ldots, |\,\mathrm{Le}(B_\ell)|\}$$

or $k \leq \ell$ and

$$\max\{|\,\mathrm{Le}(A_1)|, \ldots, |\,\mathrm{Le}(A_k|)\} \leq \min\{|\,\mathrm{Le}(B_1)|, \ldots, |\,\mathrm{Le}(B_\ell)|\}.$$

Proof. The proof is similar to the one for the Wiener index, using $|\operatorname{Le}(.)|$ instead of $|V(.)|$. ■

As we can see T is then ρ-exchange extremal, where $\rho = |\operatorname{Le}(.)|$. Moreover, if $T = [T_1, \ldots, T_k]$, then

$$|\operatorname{Le}(T)| = \begin{cases} \sum_{i=1}^{k} |\operatorname{Le}(T_i)|, & \text{if } |V(T)| \neq 1 \\ 1, & \text{otherwise.} \end{cases} \tag{6.3.6}$$

The function in (6.3.6) satisfies (6.1.1) and is increasing on any of its components and under addition of further variables. Unfortunately, (6.2.1) does not hold with strict inequality, in fact $|\operatorname{Le}(P_n)| = |\operatorname{Le}(\bullet)| = 1$. This implies that the tree satisfying Lemma 6.3.3 is not unique. The greedy tree is still optimal, but it is not the only tree that minimizes TW.

Theorem 6.3.4 ([55]). *The greedy tree is one of the trees that minimizes the terminal Wiener index $TW(T)$ among all trees with the same degree sequence.*

Example 6.3.5. Let us consider trees with degree sequence $(3,2,2,2,2,2,1,1,1)$.

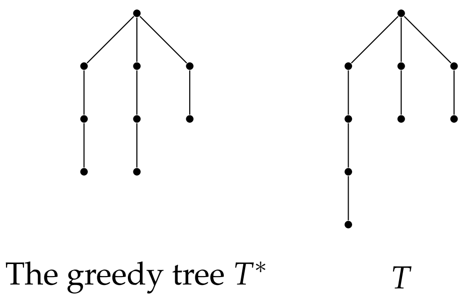


Figure 6.5: Optimal trees for the terminal Wiener index.

Let us compute the terminal Wiener index of T^* and T. $TW(T^*) = 6 + 5 + 5 = 16$ and $TW(T) = 6 + 6 + 4 = 16$, hence T^* and T have the same terminal Wiener index. Both trees satisfy Lemma 6.3.3.

6.3.3 The number of subtrees

Let T be a tree. The number of subtrees of T is denoted by $F(T)$ and the number of subtrees of T containing v is denoted by $f_T(v)$.

Lemma 6.3.6. *Let T be a tree such that $F(T) \geq F(T')$ for every T' with the same degree sequence. For any complete branches $A = [A_1, \ldots, A_k]$ and $B = [B_1, \ldots, B_\ell]$ in T, we have either*

$k \geq \ell$ and

$$\min\{f_{A_1}(\mathrm{r}(A_1)), \ldots, f_{A_k}(\mathrm{r}(A_k))\} \geq \max\{f_{B_1}(\mathrm{r}(B_1)), \ldots, f_{B_\ell}(\mathrm{r}(B_\ell))\}$$

or $k \leq \ell$ and

$$\max\{f_{A_1}(\mathrm{r}(A_1)), \ldots, f_{A_k}(\mathrm{r}(A_k))\} \leq \min\{f_{B_1}(\mathrm{r}(B_1)), \ldots, f_{B_\ell}(\mathrm{r}(B_\ell))\}.$$

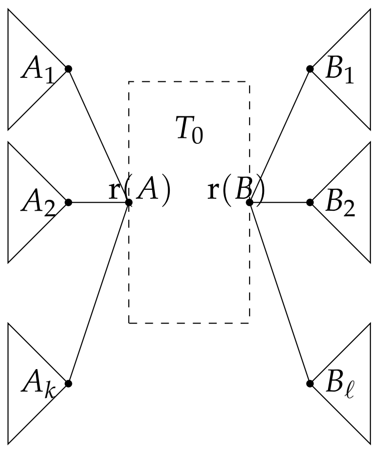


Figure 6.6: Decomposition of T in the proof of Lemma 6.3.6.

Proof. We may decompose T as in Figure 6.6 for some T_0. Let us define the following quantities:

- $F_{00}(T_0)$: number of subtrees of T_0 which contain neither $\mathrm{r}(A)$ nor $\mathrm{r}(B)$.
- $F_{10}(T_0)$: number of subtrees of T_0 which contain $\mathrm{r}(A)$ but not $\mathrm{r}(B)$.
- $F_{01}(T_0)$: number of subtrees of T_0 which contain $\mathrm{r}(B)$ but not $\mathrm{r}(A)$.
- $F_{11}(T_0)$: number of subtrees of T_0 which contain both $\mathrm{r}(A)$ and $\mathrm{r}(B)$.

The number of subtrees of T is given by:

$$\begin{aligned}F(T) = F_{00}(T_0) &+ \sum_{i=1}^{k} F(A_i) + \sum_{i=1}^{\ell} F(B_i)\\ &+ F_{01}(T_0)\prod_{i=1}^{\ell}\left(1+f_{B_i}(\mathrm{r}(B_i))\right) + F_{10}(T_0)\prod_{i=1}^{k}\left(1+f_{A_i}(\mathrm{r}(A_i))\right)\\ &+ F_{11}(T_0)\prod_{i=1}^{\ell}\left(1+f_{B_i}(\mathrm{r}(B_i))\right)\prod_{i=1}^{k}\left(1+f_{A_i}(\mathrm{r}(A_i))\right)\\ &= A_T(A_1,\ldots,A_k,B_1,\ldots,B_\ell) + B_T,\end{aligned}$$

where

$$\begin{aligned}A_T &= F_{01}(T_0)\prod_{i=1}^{\ell}\left(1+f_{B_i}(\mathrm{r}(B_i))\right) + F_{10}(T_0)\prod_{i=1}^{k}\left(1+f_{A_i}(\mathrm{r}(A_i))\right)\\ B_T &= F_{00}(T_0) + \sum_{i=1}^{k} F(A_i) + \sum_{i=1}^{\ell} F(B_i)\\ &\quad + F_{11}(T_0)\prod_{i=1}^{\ell}\left(1+f_{B_i}(\mathrm{r}(B_i))\right)\prod_{i=1}^{k}\left(1+f_{A_i}(\mathrm{r}(A_i))\right).\end{aligned}$$

As we can see, B_T is not affected by any rearrangements of A_i's and B_i's. So the maximality of $F(T)$ depends only on A_T.

Since all the quantities involved are positive, by the rearrangement inequality, we obtain the maximum of A_T if either $F_{01}(T_0) \leq F_{10}(T_0)$, $k \geq \ell$ and

$$\min\{f_{A_1}(\mathrm{r}(A_1)),\ldots,f_{A_k}(\mathrm{r}(A_k))\} \geq \max\{f_{B_1}(\mathrm{r}(B_1)),\ldots,f_{B_\ell}(\mathrm{r}(B_\ell))\}$$

or $F_{01}(T_0) \geq F_{10}(T_0)$, $k \leq \ell$ and

$$\max\{f_{A_1}(\mathrm{r}(A_1)),\ldots,f_{A_k}(\mathrm{r}(A_k))\} \leq \min\{f_{B_1}(\mathrm{r}(B_1)),\ldots,f_{B_\ell}(\mathrm{r}(B_\ell))\}.$$

■

We observe that T is ρ-exchange extremal, where $\rho(T) = f_T(\mathrm{r}(T))$. Besides, if $T = [T_1,\ldots,T_k]$, then

$$f_T(\mathrm{r}(T)) = \prod_{i=1}^{k}\left(1+f_{T_i}(\mathrm{r}(T_i))\right), \tag{6.3.7}$$

which is increasing in any of its coordinates and under addition of further coordinates, besides $f_T(\bullet) = 1$ is indeed the unique minimum. Thus, by using Theorem 6.2.3, we get

Theorem 6.3.7 ([3, 74]). *Given a degree sequence, the greedy tree maximizes the number of subtrees.*

6.3.4 Rooted spanning forests, incidence energy, Laplacian-like energy

Let $rs(T)$ be the number of rooted spanning forests in a tree T (i.e., spanning forests where each component is rooted at one of its vertices). It is well-known that $rs(T) = det(L(T) + I)$ (see Proposition 2.4.16), where $L(T)$ is the Laplacian matrix of T and I is the identity matrix.

More generally, if each rooted spanning forest F is given a weight $x^{\gamma(F)}$, where $\gamma(F)$ is the number of components of F, then we get $det(L(T) + xI)$. The following considerations apply to this generalisation as well.

To avoid confusion as we consider rooted trees, we will refer to “marked" spanning forests rather than rooted spanning forests, and call the components' roots “markers".

We define an auxiliary quantity for rooted trees, which is denoted $s(T)$. This counts rooted spanning forests in which the root of T is also a marker of one of the forest's components. Let us consider the following ratio

$$\rho(T) = \frac{rs(T)}{rs(T) + s(T)}.$$

Note that $s(T)$ also counts a different quantity: spanning forests of T where all components except the one containing T's root have a marker. The main observation is that we have an exchange-extremal lemma.

Lemma 6.3.8. *Let T be a tree such that $rs(T) \leq rs(T')$ for any T' with the same degree sequence. For any complete branches $A = [A_1, \ldots, A_k]$ and $B = [B_1, \ldots, B_\ell]$ in T, we have either*

$k \geq \ell$ and

$$\min\{\rho(A_1), \ldots, \rho(A_k)\} \geq \max\{\rho(B_1), \ldots, \rho(B_\ell)\}$$

or $k \leq \ell$ and

$$\max\{\rho(A_1), \ldots, \rho(A_k)\} \leq \min\{\rho(B_1), \ldots, \rho(B_\ell)\}.$$

Proof. Let T have a decomposition as in Figure 6.6. Let us find an expression for $rs(T)$. There are several possibilities for the spanning forest that a marked spanning forest of T induces on T_0.

- $\mathrm{r}(T_1)$ and $\mathrm{r}(T_2)$ belong to components that have a marker in H (possibly the same component). The spanning forests induced in the A_i's and B_i's are either fully marked or marked except for the root' s component (which is joined to the component of $\mathrm{r}(T_1)$ or $\mathrm{r}(T_2)$ in T_0).

  Thus the number of possibilities in this case is

$$a \cdot \prod_{i=1}^{k}(rs(A_i) + s(A_i)) \prod_{j=1}^{\ell}(rs(B_j) + s(B_j)),$$

  for some number a which depends on T_0.

- $\mathrm{r}(T_1)$ and $\mathrm{r}(T_2)$ belong to the same component, but this component does not have a marker in T_0. In this case, the marker of $\mathrm{r}(T_1)$'s and $\mathrm{r}(T_2)$'s component lies in one of the A_i's or B_j's. So we have to choose exactly one of them and replace the factor $rs(.) + s(.)$ by $rs(.)$. This gives a contribution of

$$b \cdot \prod_{i=1}^{k}(rs(A_i) + s(A_i)) \prod_{j=1}^{\ell}(rs(B_j) + s(B_j))$$
$$\left(\sum_{i=1}^{k} \frac{rs(A_i)}{rs(A_i) + s(A_i)} + \sum_{j=1}^{\ell} \frac{rs(B_j)}{rs(B_j) + s(B_j)}\right),$$

  for some b which depends on T_0.

- $\mathrm{r}(T_1)$ and $\mathrm{r}(T_2)$ lie in different components, both have markers outside of T_0. Now, one of the A_i's has to contain the marker of $\mathrm{r}(T_1)$'s component, and one of the B_j's the marker of $\mathrm{r}(T_2)$'s component. For this case we get

$$c \cdot \prod_{i=1}^{k}(rs(A_i) + s(A_i)) \prod_{j=1}^{\ell}(rs(B_j) + s(B_j))$$
$$\left(\sum_{i=1}^{k} \frac{rs(A_i)}{rs(A_i) + s(A_i)}\right) \left(\sum_{j=1}^{\ell} \frac{rs(B_j)}{rs(B_j) + s(B_j)}\right),$$

for some c which depends on T_0.

- $\mathrm{r}(T_1)$ and $\mathrm{r}(T_2)$ lie in different components, one has a marker in T_0, the other does not.

  Using a similar reasoning as before, we get

$$d_1 \cdot \prod_{i=1}^{k}(rs(A_i)+s(A_i))\prod_{j=1}^{\ell}(rs(B_j)+s(B_j)) \cdot \sum_{i=1}^{k}\frac{rs(A_i)}{rs(A_i)+s(A_i)}$$
$$+ d_2 \cdot \prod_{i=1}^{k}(rs(A_i)+s(A_i))\prod_{j=1}^{\ell}(rs(B_j)+s(B_j)) \cdot \sum_{j=1}^{\ell}\frac{rs(B_j)}{rs(B_j)+s(B_j)},$$

  for certain numbers d_1 and d_2 that depend on T_0.

The total number $rs(T)$ of marked spanning forests is the sum of all these terms. We can take out a factor:

$$\prod_{i=1}^{k}(rs(A_i)+s(A_i))\prod_{j=1}^{\ell}(rs(B_j)+s(B_j))$$
$$\Bigg[a+(b+d_1)\sum_{i=1}^{k}\frac{rs(A_i)}{rs(A_i)+s(A_i)}+(b+d_2)\sum_{j=1}^{\ell}\frac{rs(B_j)}{rs(B_j)+s(B_j)}$$
$$+c\left(\sum_{i=1}^{k}\frac{rs(A_i)}{rs(A_i)+s(A_i)}\right)\left(\sum_{j=1}^{\ell}\frac{rs(B_j)}{rs(B_j)+s(B_j)}\right)\Bigg].$$

The product $\prod_{i=1}^{k}(rs(A_i)+s(A_i))\prod_{j=1}^{\ell}(rs(B_j)+s(B_j))$ remains constant when the A_i's and B_j's are rearranged, as does the sum

$$S=\sum_{i=1}^{k}\frac{rs(A_i)}{rs(A_i)+s(A_i)}+\sum_{j=1}^{\ell}\frac{rs(B_j)}{rs(B_j)+s(B_j)}$$
$$=\sum_{i=1}^{k}\rho(A_i)+\sum_{j=1}^{\ell}\rho(B_j).$$

Write $x=\sum_{i=1}^{k}\rho(A_i)$. In order to minimise $rs(T)$, we have to minimise

$$a+(b+d_1)x+(b+d_2)(S-x)+cx(S-x).$$

This is a concave function of x, so the minimum is attained when x is either as large or as small as possible.

Thus, for our situation, $rs(T)$ attains its minimum if either
$k \geq \ell$ and

$$\min\{\rho(A_1), \ldots, \rho(A_k)\} \geq \max\{\rho(B_1), \ldots, \rho(B_\ell)\}$$

or $k \leq \ell$ and

$$\max\{\rho(A_1), \ldots, \rho(A_k)\} \leq \min\{\rho(B_1), \ldots, \rho(B_\ell)\}.$$

■

Moreover, the quantity ρ can be determined recursively as follows. If $T = [T_1, \ldots, T_k]$, we easily see that

$$rs(T) = \prod_{i=1}^{k} (rs(T_i) + s(T_i)) \left(1 + \sum_{i=1}^{k} \frac{rs(T_i)}{rs(T_i) + s(T_i)}\right),$$

and

$$s(T) = \prod_{i=1}^{k} (rs(T_i) + s(T_i))$$

using similar arguments as before. Hence

$$\rho(T) = \frac{1 + \sum_{i=1}^{k} \rho(T_i)}{2 + \sum_{i=1}^{k} \rho(T_i)}. \tag{6.3.8}$$

Furthermore, for the general case where each rooted spanning forest is given a weight $x^{\gamma(F)}$ according to the number γ of components, we denote by $rs(T, x)$ the number of rooted spanning forests, and $s(T, x)$ the analogous quantity where the root is also a marker. As before, we set

$$\rho(T, x) = \frac{rs(T, x)}{rs(T, x) + s(T, x)}.$$

In the same way as for the simple case where $x = 1$, with careful attention to the weights we have the following recursions.

$$rs(T, x) = x^{1-k} \prod_{i=1}^{k} (x\, rs(T_i, x) + s(T_i, x)) \left(1 + \sum_{i=1}^{k} \frac{rs(T_i, x)}{x\, rs(T_i, x) + s(T_i, x)}\right),$$

and

$$s(T,x) = x^{1-k}\prod_{i=1}^{k}(x\,rs(T_i,x)+s(T_i,x)).$$

Thus,

$$\begin{aligned}\rho(T,x) =& \frac{1+\sum_{i=1}^{k}\frac{rs(T_i,x)}{x\,rs(T_i,x)+s(T_i,x)}}{2+\sum_{i=1}^{k}\frac{rs(T_i,x)}{x\,rs(T_i,x)+s(T_i,x)}}\\ =& \frac{1+\sum_{i=1}^{k}\frac{1}{x-1+\rho(T_i,x)^{-1}}}{2+\sum_{i=1}^{k}\frac{1}{x-1+\rho(T_i,x)^{-1}}}. \end{aligned} \tag{6.3.9}$$

The functions in (6.3.8) and in (6.3.9) are increasing in any of their coordinates and under addition of further coordinates, moreover $\rho(\bullet) = \rho(\bullet, x) = \frac{1}{2}$ is the unique minimum. So, we may use Theorem 6.2.3 to obtain

Theorem 6.3.9. *For any tree T with given degree sequence D,*

$$rs(T) \geq rs(G(D)),$$

where $G(D)$ is the greedy tree with the same degree sequence.

More generally, for $x > 0$,

$$rs(T,x) \geq rs(G(D),x).$$

Let T be a tree and $c_k(T)$ be the number of k-rooted spanning forests of T. It is well-known that the $c_k(T)$'s are also the coefficients of $det(L(T)+xI)$.

Let us consider the following lemma that links $c_k(T)$ to the matchings of of the subdivision graph of T.

Lemma 6.3.10 ([75])**.** *Let T be a tree of order n and $S(T)$ its corresponding subdivision graph. Then*

$$c_k(T) = \mathrm{m}(S(T),k), \quad k = 0,\dots,n,$$

where $\mathrm{m}(S(T),k)$ is the number of k-matchings of $S(T)$.

Let $\mathrm{M}(T,x)$ be the matching generating polynomial of T; then Lemma 6.3.10 implies $rs(T,x) = \mathrm{M}(S(T),x)$. Thus, from Theorem 6.3.9, we obtain

Corollary 6.3.11. *For any tree T with given degree sequence D, and for $x > 0$,*

$$\mathrm{M}(S(T),x) \geq \mathrm{M}(S(G(D)),x).$$

Now, let us consider other quantities related to the Laplacian polynomial. Let $\mu_1, \mu_2, \ldots, \mu_n$ be the zeros of the Laplacian polynomial $\mathrm{L}(G, x)$, the "Laplacian-energy-like" invariant, introduced by Liu and Liu in [48], is defined as:

$$\mathrm{LEL}(G) = \sum_{i=1}^{n} \sqrt{\mu_i}. \tag{6.3.10}$$

On the other hand, Jooyandeh and al. [39] proposed the "incidence energy" as the energy of the incidence matrix of a graph.

Let G be a graph of order n and size m, such that $V(G) = \{v_1, \ldots, v_n\}$ and $E(G) = \{e_1, \ldots, e_m\}$. The incidence matrix of G is an $n \times m$ matrix whose (i, j)-entry is either 1 if v_i is an endpoint of e_j and 0 otherwise.

Let $\mu_1^+, \mu_2^+, \ldots, \mu_n^+$ be the eigenvalues of the signless Laplacian matrix $L^+(G) = D(G) + A(G)$. Then, it has been shown in [28] that the incidence energy is:

$$\mathrm{IE}(G) = \sum_{i=1}^{n} \sqrt{\mu_i^+}. \tag{6.3.11}$$

Furthermore, the following is well-known ([11]):

Lemma 6.3.12. *The spectra of $L(G)$ and $L^+(G)$ coincide if and only if the graph G is bipartite.*

Therefore, we may deduce from (6.3.10) and (6.3.11) that LEL and IE coincide for bipartite graphs. Furthermore, from the same paper [28], we have the following result.

Lemma 6.3.13. *For any tree T, we have*

$$\mathrm{LEL}(T) = \mathrm{IE}(T) = \frac{1}{2}\,\mathrm{E}(S(T)),$$

where $\mathrm{E}(S(T))$ is the energy of the subdivision graph of T.

Furthermore, we can write the energy of a tree in terms of its matchings by means of the Coulson-integral formula [29]:

$$\mathrm{E}(T) = \frac{2}{\pi} \int_0^\infty \frac{1}{x^2} \ln\left(\sum_k \mathrm{m}(T, k) x^{2k}\right) dx. \tag{6.3.12}$$

Corollary 6.3.14. *Given a degree sequence, the incidence energy* IE *and the Laplacian-like energy* LEL *are minimized by the greedy tree.*

Proof. Let T be a tree and $S(T)$ its subdivision graph. Using Lemma 6.3.13 and Equation (6.3.12), we obtain:

$$\mathrm{LEL}(T) = \mathrm{IE}(T) = \frac{1}{\pi}\int_0^{\infty} \frac{1}{x^2} \ln\left(\sum_k \mathrm{m}(S(T),k)x^{2k}\right) dx.$$

As we can see, LEL and IE are increasing functions in terms of the sum $\sum_k \mathrm{m}(S(T),k)x^{2k}$, which corresponds to $\mathrm{M}(S(T),x^2)$. Now, we get the result by using Corollary 6.3.11. ∎

6.4 Decreasing recurrence rule f_ρ

In this section, we assume that the function f_ρ satisfies (6.1.1) and is strictly decreasing (decreasing with respect to any of its variables and decreasing by adding further elements), and

$$\rho(\bullet) > \rho(B) \tag{6.4.1}$$

for all rooted trees B with $|V(B)| > 1$. The following definitions are taken from [1].

Definition 6.4.1. A complete branch $B = [B_1, \ldots, B_k]$ of a tree T is a *pseudo-leaf* if $|V(B_1)| = |V(B_2)| = \cdots = |V(B_k)| = 1$.

We denote by $[d]$ a pseudo-leaf branch with d vertices.

Definition 6.4.2. Let $(d_1, \ldots, d_t, 1, \ldots, 1)$ be the degree sequence of a tree T, where $d_j \geq 2$ for $1 \leq j \leq t$. The t-tuple $(d_1, \ldots, d_t)$ is called the *reduced degree sequence* of T.

For every tree T with reduced degree sequence $(d_1, \ldots, d_t)$ and k leaves, the Handshake lemma gives $k + \sum_{j=1}^{t} d_j = 2(n-1)$, where $n = k + t$ is the order of T. It implies that two trees with the same reduced degree sequence have the same number of leaves, therefore they have the same degree sequence. We assume that the d_i's are in a non-increasing order, i.e., $d_1 \geq d_2 \geq \cdots \geq d_t$.

Definition 6.4.3. Let $(d_1, \ldots, d_t)$ be a reduced degree sequence of a tree. If $t \leq d_t + 1$, then $\mathcal{M}(d_1, \ldots, d_t)$ is the tree obtained by merging the root of each of $[d_1], \ldots, [d_{t-1}]$ with a leaf of $[1 + d_t]$, respectively. We label selected vertices as shown in Figure 6.7, in such a way that

$$d(v_i) \leq d(v_j) \quad \text{if } i < j. \tag{6.4.2}$$

At this point all non-leaf vertices are labelled.

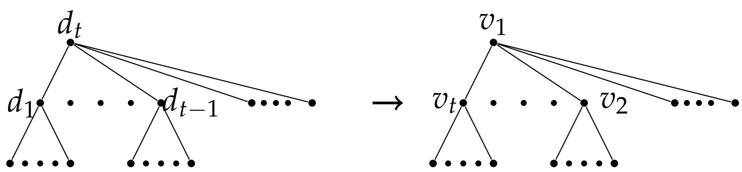


Figure 6.7: Labelling of the vertices.

On the other hand, if $t \geq d_t + 2$, we construct $\mathcal{M}(d_1, \ldots, d_t)$ recursively: let ℓ be the greatest integer such that v_ℓ is a label in $\mathcal{M}(d_{d_t}, \ldots, d_{t-1})$. Let s be the smallest integer such that v_s is adjacent to a leaf in $\mathcal{M}(d_{d_t}, \ldots, d_{t-1})$. Let $R_{d_t} = [[d_1], \ldots, [d_{d_t-1}]]$, where the pseudo-leaves are labelled $v_{\ell+1}, \ldots,$ $v_{\ell+d_t-1}$ still respecting 6.4.2. $\mathcal{M}(d_1, \ldots, d_t)$ is the tree obtained by merging the root of R_{d_t} to a leaf adjacent to v_s.

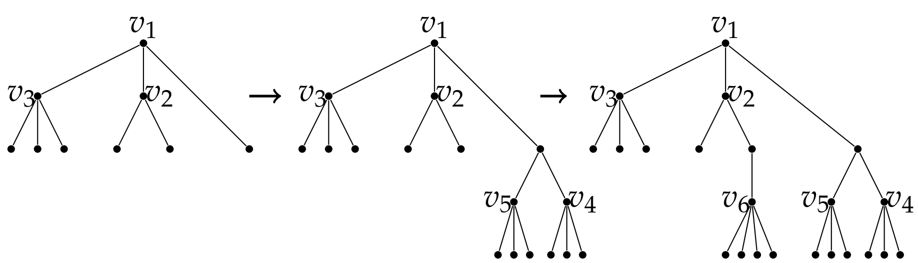


Figure 6.8: Construction of $\mathcal{M}(5, 4, 4, 4, 3, 3, 3, 2)$.

If D is the degree sequence associated to the reduced degree sequence D', we use both $\mathcal{M}(D)$ and $\mathcal{M}(D')$ to denote the same graph.

Let T be a rooted tree. We set $\mathrm{M}(T)$ to be the number of matchings in T, and $\mathrm{M}_0(T)$ the number of matchings in T that do not cover $\mathrm{r}(T)$. We consider the following ratio:

$$\rho_1(T) = \frac{\mathrm{M}_0(T)}{\mathrm{M}(T)}.$$

As a special case (for $x = 1$) of Theorem 22 in [1], the following is known:

Theorem 6.4.4 ([1])**.** *For any given degree sequence D, the unique ρ_1-exchange-extremal tree with degree sequence D is $\mathcal{M}(D)$.*

Analogously to Theorem 6.2.3, we may obtain the following result.

Theorem 6.4.5. *Let ρ be an invariant of rooted trees that satisfies* (6.1.1) *and* (6.4.1) *for a decreasing f_ρ. The unique ρ-exchange-extremal tree with degree sequence D is $\mathcal{M}(D)$.*

Proof. To prove the theorem, we only need to show that for any complete branches A and B in T, $\rho(A) \le \rho(B)$ if and only if $\rho_1(A) \le \rho_1(B)$.

We reason by induction on $\max\{h(A), h(B)\}$. If $\max\{h(A), h(B)\} = 0$, then $h(A) = h(B) = 0$ and A and B are isomorphic rooted trees and the claim holds trivially. Assume that it holds whenever $\max\{h(A), h(B)\} \le t$, for some $t \ge 0$. Now, consider the case where $\max\{h(A), h(B)\} = t + 1$. We assume there exist two complete branches A and B in T such that $\max\{h(A), h(B)\} = t + 1$ and $\rho(A) \ge \rho(B)$. Since f_ρ and f_{ρ_1} are increasing and $\rho(\bullet)$, $\rho_1(\bullet)$ are the respective maxima, we have $1 \notin \{|V(A), V(B)|\}$. Write $A = [A_1, \ldots, A_k]$ and $B = [B_1, \ldots, B_\ell]$.

If $k \ge \ell$, by Definition 6.1.2, we have

$$\min\{\rho(A_i) : 1 \le i \le k\} \ge \max\{\rho(B_i) : 1 \le i \le \ell\},$$

then by the induction hypothesis, we have

$$\min\{\rho_1(A_i) : 1 \le i \le k\} \ge \max\{\rho_1(B_i) : 1 \le i \le \ell\}.$$

Thus $\rho_1(A) \ge \rho_1(B)$.

On the other hand, if $k \le \ell$, by Definition 6.1.2 again, we have

$$\max\{\rho(A_i) : 1 \le i \le k\} \le \max\{\rho(B_i) : 1 \le i \le \ell\},$$

then $\rho(A) \le \rho(B)$ since f_ρ is increasing, so $\rho(A) = \rho(B)$. For this to hold, we must have $k = \ell$ and $\rho(A_1) = \cdots = \rho(A_k) = \rho(B_1) = \cdots = \rho(B_\ell)$. By the induction hypothesis, this implies $\rho_1(A_1) = \cdots = \rho_1(A_k) = \rho_1(B_1) = \cdots = \rho_1(B_\ell)$, so $\rho_1(A) = \rho_1(B)$.

Thus we have shown that $\rho(A) \ge \rho(B)$ implies $\rho_1(A) \ge \rho_1(B)$ and the converse is analogous.

∎

6.5 Applications of Theorem 6.4.5

6.5.1 Matching polynomial, Hosoya index, energy

Let T be a rooted tree, $\mathrm{m}_1(T,k)$ be the number of k-matchings containing the root and $\mathrm{m}_0(T,k)$ be the number of k-matchings not containing the root. We defined earlier their corresponding polynomials:

$$\mathrm{M}_i(T,x) = \sum_k \mathrm{m}_i(T,k)x^k, \quad \text{for} \quad i \in \{0,1\}.$$

Note that the matching polynomial is $\mathrm{M}(T,x) = \mathrm{M}_0(T,x) + \mathrm{M}_1(T,x)$. Recall the ratio:

$$\tau(T,x) = \frac{\mathrm{M}_0(T,x)}{\mathrm{M}(T,x)}.$$

Lemma 6.5.1 ([1]). *Let $x > 0$, and T be a tree such that $\mathrm{M}(T,x) \leq \mathrm{M}(T',x)$ for every T' with the same degree sequence. For any complete branches $A = [A_1,\ldots,A_k]$ and $B = [B_1,\ldots,B_\ell]$, we have either*

$k \geq \ell$ and

$$\min\{\tau(A_j,x) : 1 \leq j \leq k\} \geq \max\{\tau(B_j,x) : 1 \leq j \leq \ell\}$$

or $k \leq \ell$ and

$$\max\{\tau(A_j,x) : 1 \leq j \leq k\} \leq \min\{\tau(B_j,x) : 1 \leq j \leq \ell\}.$$

The tree that minimizes the matching polynomial $\mathrm{M}(T,x)$ for some $x > 0$ is $\tau(.,x)$-exchange-extremal. Thus

Theorem 6.5.2 ([1]). *Let $x > 0$. If T is a tree with degree sequence D, then*

$$\mathrm{M}(T,x) \geq \mathrm{M}(\mathcal{M}(D),x).$$

The Hosoya index of a graph G is the total number of matchings of G.

Corollary 6.5.3 ([1]). *Given a degree sequence D of a tree, the Hosoya index is minimized by $\mathcal{M}(D)$.*

In view of the relation between the energy and the matching polynomial in Equation (6.3.12), we also get:

Corollary 6.5.4 ([1]). *Given a degree sequence D of a tree, the energy is minimized by $\mathcal{M}(D)$.*

6.5.2 Independent sets

Let T be a rooted tree, $\sigma_1(T)$ be the number of independent sets of T which contain the root and $\sigma_0(T)$ be the number of independent sets of T which do not contain the root. As we can see, the total number of independent sets is $\sigma(T) = \sigma_0(T) + \sigma_1(T)$. Let us define the ratio $\rho(T) = \frac{\sigma_0(T)}{\sigma(T)}$.

Lemma 6.5.5 ([33]). *Let $T = [T_1, \ldots, T_k]$, then*

$$\begin{aligned} \sigma_0(T) &= \prod_{j=1}^{k} \sigma(T_j), \\ \sigma_1(T) &= \prod_{j=1}^{k} \sigma_0(T_j), \\ \rho(T) &= \frac{1}{1 + \prod_{j=1}^{k} \rho(T_j)}. \end{aligned} \tag{6.5.1}$$

Lemma 6.5.6 (Cf [33]). *Let T be a tree such that $\rho(T) \geq \rho(T')$ for every T' with the same degree sequence. For any complete branches $A = [A_1, \ldots, A_k]$ and $B = [B_1, \ldots, B_\ell]$, we have either*

$k \geq \ell$ and

$$\min\{\rho(A_j) : 1 \leq j \leq k\} \geq \max\{\rho(B_j) : 1 \leq j \leq \ell\}$$

or $k \leq \ell$ and

$$\max\{\rho(A_j) : 1 \leq j \leq k\} \leq \min\{\rho(B_j) : 1 \leq j \leq \ell\}.$$

The tree that maximizes the number of independent sets, also called Merrifield-Simmon index, satisfies the ρ-exchange extremal property. Moreover, from (6.5.1), f_ρ is decreasing on any of its components. Applying Theorem 6.4.5, we get

Theorem 6.5.7 ([1]). *Given a degree sequence D, the Merrifield-Simmon index is maximized by $\mathcal{M}(D)$.*

6.5.3 Solvability

Let $G = (V(G), E(G))$ be a graph and $v \in V(G)$. The open neighbourhood of v denoted $N(v)$ is the set $\{u \in V(G) | uv \in E(G)\}$, and the closed neighbourhood of v is $N[v] = N(v) \cup \{v\}$.

We are concerned with domination problems with parity constraints. We are looking for a set of vertices satisfying, for each of the vertices of the graph, one of four possible conditions: the open/closed neighbourhood has to contain an even/odd number of vertices in S. This can be stated in terms of matrix algebra. Let A and $A+I$ be the open neighbourhood matrix (the adjacency matrix) and the closed neighbourhood matrix respectively. Furthermore, we consider a vector $a \in \{0,1\}^{V(G)}$ as a representation for the neighbourhood information, i.e., whether the open or closed neighbourhood is of interest for this vertex, and $b \in \{0,1\}^{V(G)}$ represents the prescribed parities. Using these notations, our problem can be written as:

$$(A + diag(a))x = b, \tag{6.5.2}$$

which is an equation over the field $\mathbb{F}_2$.

The *solvability* of G, denoted $s(G)$, is the number of instances where (6.5.2) can be solved. More explicitly, we are interested in the number of pairs (a,b) such that there exists a vector x satisfying the system of linear equations in (6.5.2).

Lemma 6.5.8 ([32]). *Let T be a rooted tree with root v. If $T_1,\dots,T_k$ are the branches of T and $v_1,\dots,v_k$ their respective roots, then*

$$s(T) = 8\prod_{i=1}^{k} s(T_i) - 5\prod_{i=1}^{k} t(T_i,v_i),$$
$$t(T,v) = 8\prod_{i=1}^{k} s(T_i) - 6\prod_{i=1}^{k} t(T_i,v_i),$$

where $t(T,v)$ is an auxiliary parameter depending on the root v.

Let $\rho(T,v)$ be the ratio $\rho = \frac{t(T,v)}{s(T)}$. If $T = [T_1,\dots,T_k]$, then by Lemma 6.5.8 we have:

$$\rho(T,v) = \frac{1}{1 + \frac{1}{8\prod_{i=1}^{k}\frac{1}{\rho(T_i,v_i)} - 6}}. \tag{6.5.3}$$

Lemma 6.5.9. *Let T be a tree such that $s(T) \le s(T')$ for every T' with the same degree sequence. For any complete branches $A = [A_1,\dots,A_k]$ and $B = [B_1,\dots,B_\ell]$, we have either*

$k \ge \ell$ *and* $\min\{\rho(A_j) : 1 \le j \le k\} \ge \max\{\rho(B_j) : 1 \le j \le \ell\}$

or $k \le \ell$ *and* $\max\{\rho(A_j) : 1 \le j \le k\} \le \min\{\rho(B_j) : 1 \le j \le \ell\}$.

Proof. Let $\mathrm{r}(A) = u_0u_1\dots u_t = \mathrm{r}(B)$ be the path between $\mathrm{r}(A)$ and $\mathrm{r}(B)$. For $0 < j < t$, let U_j be the subtree containing u_j when we remove all the edges of the path $P_T(\mathrm{r}(A),\mathrm{r}(B))$. Furthermore, for each j, we have $U_j = [U_j^1,\dots,U_j^{rd(U_j)}]$. We also denote by X_j the subtree containing u_j by removing the edge $u_{j-1}u_j$. For ease of notation, we will write $t(T,\mathrm{r}(A)), t(U_i,u_i)$ and $t(X_i,u_i)$ as $t(T), t(U_i)$ and $t(X_i)$, respectively. Using Lemma 6.5.8, we can write $s(T)$ and $t(T)$ in terms of matrices as follows:

$$\begin{pmatrix} s(T) \\ t(T) \end{pmatrix} = \begin{pmatrix} 8\prod_{i=1}^k s(A_i) & -5\prod_{i=1}^k t(A_i) \\ 8\prod_{i=1}^k s(A_i) & -6\prod_{i=1}^k t(A_i) \end{pmatrix} \begin{pmatrix} s(X_1) \\ t(X_1) \end{pmatrix}.$$

Moreover, for $0 < j < t$, we have

$$\begin{pmatrix} s(X_j) \\ t(X_j) \end{pmatrix} = \begin{pmatrix} 8\prod_{i=1}^{rd(U_j)} s(U_j^i) & -5\prod_{i=1}^{rd(U_j)} t(U_j^i) \\ 8\prod_{i=1}^{rd(U_j)} s(U_j^i) & -6\prod_{i=1}^{rd(U_j)} t(U_j^i) \end{pmatrix} \begin{pmatrix} s(X_{j+1}) \\ t(X_{j+1}) \end{pmatrix}.$$

Let us denote the matrix $\begin{pmatrix} 8\prod_{i=1}^{rd(U_j)} s(U_j^i) & -5\prod_{i=1}^{rd(U_j)} t(U_j^i) \\ 8\prod_{i=1}^{rd(U_j)} s(U_j^i) & -6\prod_{i=1}^{rd(U_j)} t(U_j^i) \end{pmatrix}$ by M_j. Then,

$$\begin{pmatrix} s(T) \\ t(T) \end{pmatrix} = \begin{pmatrix} 8\prod_{i=1}^k s(A_i) & -5\prod_{i=1}^k t(A_i) \\ 8\prod_{i=1}^k s(A_i) & -6\prod_{i=1}^k t(A_i) \end{pmatrix} M \begin{pmatrix} s(B) \\ t(B) \end{pmatrix},$$

where $M = M_0 \times M_1 \times M_2 \times \cdots M_{t-1}$, M_0 being the identity matrix. If we set $M = \begin{pmatrix} M_{00} & M_{01} \\ M_{10} & M_{11} \end{pmatrix}$, then we can write the solvability of T as

$$\begin{aligned}
&\prod_{i=1}^k s(A_i)\prod_{i=1}^{\ell} s(B_i)(64M_{00}+64M_{01}) + \prod_{i=1}^k s(A_i)\prod_{i=1}^{\ell} t(B_i)(-40M_{00}-48M_{01}) \\
&\quad + \prod_{i=1}^k t(A_i)\prod_{i=1}^{\ell} s(B_i)(-40M_{10}-40M_{11}) + \prod_{i=1}^k t(A_i)\prod_{i=1}^{\ell} t(B_i)(25M_{10}+30M_{11}) \\
&= \prod_{i=1}^k s(A_i)\prod_{i=1}^{\ell} s(B_i)\Big[64M_{00}+64M_{01} + \prod_{i=1}^{\ell}\rho(B_i)(-40M_{00}-48M_{01}) \\
&\quad + \prod_{i=1}^k \rho(A_i)(-40M_{10}-40M_{11}) + \prod_{i=1}^k \rho(A_i)\prod_{i=1}^{\ell}\rho(B_i)(25M_{10}+30M_{11})\Big] \\
&= \prod_{i=1}^k s(A_i)\prod_{i=1}^{\ell} s(B_i)Sf(A_1,\dots,A_k,B_1,\dots,B_\ell).
\end{aligned}$$

The product $\prod_{i=1}^{k} s(A_i) \prod_{i=1}^{\ell} s(B_i)$ is invariant under any rearrangements of A_i's and B_i's, so $s(T)$ is minimal if and only if

$$Sf(A_1, \ldots, A_k, B_1, \ldots, B_\ell) \leq Sf(\pi(A_1), \ldots \pi(A_k), \pi(B_1), \ldots \pi(B_\ell))$$

for every permutation π. Moreover the sum $64M_{00} + 64M_{01} + \prod_{i=1}^{k} r(A_i) \prod_{i=1}^{\ell} r(B_i)(25M_{10} + 30M_{11})$ does not depend on the permutation. Hence Sf is minimal if $-\left(A \prod_{i=1}^{\ell} r(B_i) + B \prod_{i=1}^{k} r(A_i)\right)$, where $A = (40M_{00} + 48M_{01})$ and $B = (40M_{10} + 40M_{11})$, is minimal.

We need to show that A and B are positive. For $t = 1$, M is equal to the identity matrix. Then $A = B = 40 > 0$.

Now, for $t > 1$, let us prove by induction on t that $5M_{00} + 6M_{01}, 5M_{10} + 6M11 > 0$ and $M_{01}, M_{11} \leq 0$. Note that the positivity of $5M_{00} + 6M_{01}$ implies the positivity of A since $A = 8(5M_{00} + 6M_{01})$, and the positivity of $5M_{10} + 6M_{11}$ implies the positivity of B since $B = 8(5M_{10} + 5M_{11}) \geq 8(5M_{10} + 6M_{11})$. We will write $M(t)$ and $M_{ij}(t)$ $(i, j \in \{0, 1\})$ for the matrices M and M_{ij} corresponding to t. For $t = 2$, since for all i, $s(U_1^i) > t(U_1^i) \geq 0$, we have

$$\begin{aligned}
M_{01}(2) &= -5 \prod_{i=1}^{rd(U_1)} t(U_1^i) \leq 0, \\
M_{11}(2) &= -6 \prod_{i=1}^{rd(U_1)} t(U_1^i) \leq 0, \\
5M_{00} + 6M_{01} &= 40 \prod_{i=1}^{rd(U_1)} s(U_1^i) - 30 \prod_{i=1}^{rd(U_1)} t(U_1^i) > 0, \\
5M_{10} + 6M_{11} &= 40 \prod_{i=1}^{rd(U_1)} s(U_1^i) - 36 \prod_{i=1}^{rd(U_1)} t(U_1^i) > 0
\end{aligned}$$

Suppose that it is true for some $t \leq m$. Now, we set $t = m + 1$, and $M(m + 1) = M_0 \times M_1 \times M_2 \times \cdots M_m = M(m) \times M_m$. Therefore,

$$\begin{aligned}
M_{00}(m+1) &= 8 \prod_{i=1}^{rd(U_{m+1})} s(U_{m+1}^i)(M_{00}(m) + M_{01}(m)), \\
M_{01}(m+1) &= - \prod_{i=1}^{rd(U_{m+1})} t(U_{m+1}^i)(5M_{00}(m) + 6M_{01}(m)),
\end{aligned}$$

$$M_{10}(m+1) = 8 \prod_{i=1}^{rd(U_{m+1})} s(U^i_{m+1})(M_{10}(m) + M_{11}(m)),$$
$$M_{11}(m+1) = -\prod_{i=1}^{rd(U_{m+1})} t(U^i_{m+1})(5M_{10}(m) + 6M_{11}(m)).$$

By the induction hypothesis, we have $M_{01}(m), M_{11}(m) \leq 0$, $5M_{00}(m) + 6M_{01}(m), 5M_{10}(m) + 6M_{11}(m) > 0$. Besides, for all i, $s(U^i_{m+1}) > t(U^i_{m+1}) \geq 0$, so

$$M_{01}(m+1) \leq 0,$$
$$M_{11}(m+1) \leq 0.$$

Furthermore, with the same assumptions, we get

$$\begin{aligned}
5M_{00}(m+1) + 6M_{01}(m+1) &= 5 \times 8 \prod_{i=1}^{rd(U_{m+1})} s(U^i_{m+1})(M_{00}(m) + M_{01}(m)) \\
&\quad - 6 \prod_{i=1}^{rd(U_{m+1})} t(U^i_{m+1})(5M_{00}(m) + 6M_{01}(m)) \\
&\geq (5M_{00}(m) + 6M_{01}(m)) \\
&\quad \left(8 \prod_{i=1}^{rd(U_{m+1})} s(U^i_{m+1}) - 6 \prod_{i=1}^{rd(U_{m+1})} t(U^i_{m+1})\right) \\
&> 0, \\
5M_{10}(m+1) + 6M_{11}(m+1) &= 5 \times 8 \prod_{i=1}^{rd(U_{m+1})} s(U^i_{m+1})(M_{10}(m) + M_{11}(m)) \\
&\quad - 6 \prod_{i=1}^{rd(U_{m+1})} t(U^i_{m+1})(5M_{10}(m) + 6M_{11}(m)) \\
&\geq (5M_{10}(m) + 6M_{11}(m)) \\
&\quad \left(8 \prod_{i=1}^{rd(U_{m+1})} s(U^i_{m+1}) - 6 \prod_{i=1}^{rd(U_{m+1})} t(U^i_{m+1})\right) \\
&> 0.
\end{aligned}$$

Since $A, B, r(A_i)$'s and $r(B_i)$'s are all positive, by the rearrangement inequality, Sf is minimal if:

$A \leq B$ and $k \geq \ell$ and $\min\{\rho(A_j) : 1 \leq j \leq k\} \geq \max\{\rho(B_j) : 1 \leq j \leq \ell\}$
or $A \geq B$ and $k \leq \ell$ and $\max\{\rho(A_j) : 1 \leq j \leq k\} \leq \min\{\rho(B_j) : 1 \leq j \leq \ell\}$. ■

The tree that minimizes the solvability, satisfies the ρ-exchange-extremal property. Moreover, by (6.5.3), f_ρ is decreasing on any of its components. Applying Theorem 6.4.5, we get

Theorem 6.5.10. *Given a degree sequence of a tree D, the solvability is minimized by $\mathcal{M}(D)$.*

We have seen two similar examples, the first one for independent sets and the second one for the solvability. In each case, we were dealing with two parameters that can be computed by means of the parameters of their branches. One may wonder if we can generalise those cases. So, if we consider a rooted tree T, rooted at v, and $T_1, \dots, T_k$ the branches of T and $v_1, \dots, v_k$ their respective roots, we consider recursions of the form

$$A(T) = a \prod_{i=1}^{k} A(T_i) + b \prod_{i=1}^{k} B(T_i, v_i), \tag{6.5.4}$$

$$B(T, v) = c \prod_{i=1}^{k} A(T_i) + d \prod_{i=1}^{k} B(T_i, v_i), \tag{6.5.5}$$

where $A(T)$ and $B(T, v)$ are some parameters.

We are interested in the choice of (a, b, c, d), where A is a well-defined parameter (independent of v) and eventually extremal for the greedy tree or the tree $\mathcal{M}(D)$. We have seen already that $(1, 1, 1, 0)$ and $(8, -5, 8, -6)$ work as they are the cases for independent sets and solvability.

In order to be a proper parameter, A must not depend on the choice of the root. Hence, if we compute for example $A(P_3)$ using the centre (the vertex of degree 2) as the root, it should correspond to the case when we choose a leaf as the root. From this observation, we have the following equation that (a, b, c, d) have to satisfy:

$$(a + b - c - d)(a - c)b = 0. \tag{6.5.6}$$

The solution of (6.5.6) falls into the following cases:

- $b = 0$,

- $a = c$,
- $a + b = c + d$.

In the first case and the last case, A is actually independent of the tree but only depends on the number of vertices. Thus these cases are not really interesting. So, we focus on the case where $a = c$.

Proposition 6.5.11. *If $a = c$, then A is independent of the choice of the root.*

Proof. Let T be a tree, and u, v be some vertices of T. We are going to show that $A(T)$ is the same if we consider either u or v as the root. Without loss of generality, we may assume that $d(u, v) = 1$. Let $U_1, \ldots, U_k$ (resp. $V_1, \ldots, V_\ell$) be the branches of u not containing v (resp. the branches of v not containing u) attached to $u_1, \ldots, u_k$ (resp. $v_1, \ldots, v_\ell$). We denote by $A(T)^u$ and $A(T)^v$ the parameter $A(T)$ computed from u and v respectively. For ease of notation, we will write $B(U_i)$ (resp. $B(V_i)$) instead of $B(U_i, u_i)$ (resp. $B(V_i, v_i)$).

$$\begin{aligned}
A(T)^u &= a\prod_{i=1}^{k} A(U_i)\left(a\prod_{i=1}^{\ell} A(V_i) + b\prod_{i=1}^{\ell} B(V_i)\right) \\
&\quad + b\prod_{i=1}^{k} B(U_i)\left(a\prod_{i=1}^{\ell} A(V_i) + d\prod_{i=1}^{\ell} B(V_i)\right) \\
&= a^2\prod_{i=1}^{k} A(U_i)\prod_{i=1}^{\ell} A(V_i) + ab\prod_{i=1}^{k} A(U_i)\prod_{i=1}^{\ell} B(V_i) \\
&\quad + ab\prod_{i=1}^{k} B(U_i)\prod_{i=1}^{\ell} A(V_i) + bd\prod_{i=1}^{k} B(U_i)\prod_{i=1}^{\ell} B(V_i).
\end{aligned}$$

On the other hand,

$$\begin{aligned}
A(T)^v &= a\prod_{i=1}^{\ell} A(V_i)\left(a\prod_{i=1}^{k} A(U_i) + b\prod_{i=1}^{k} B(U_i)\right) \\
&\quad + b\prod_{i=1}^{\ell} B(V_i)\left(a\prod_{i=1}^{k} A(U_i) + d\prod_{i=1}^{k} B(U_i)\right) \\
&= a^2\prod_{i=1}^{\ell} A(V_i)\prod_{i=1}^{k} A(U_i) + ab\prod_{i=1}^{\ell} A(V_i)\prod_{i=1}^{k} B(U_i) \\
&\quad + ab\prod_{i=1}^{\ell} B(V_i)\prod_{i=1}^{k} A(U_i) + bd\prod_{i=1}^{\ell} B(V_i)\prod_{i=1}^{k} B(U_i).
\end{aligned}$$

Since the product is commutative, then $A(T)^u = A(T)^v$.

■

Now, we are interested in some combinatorial meaning of A. Let $\mathcal{C}_2(T)$ be the set of two-colorings (not necessarily proper) of T. We choose the colors to be blue and red. We have the following proposition:

Proposition 6.5.12.

$$\begin{aligned} A(T) &= \sum_{C \in \mathcal{C}_2} a^{n_R(T)} b^{k_B(T)} d^{m_B(T)}, \\ B(T,v) &= \sum_{C \in \mathcal{C}_2} a^{n_R(T)} b^{k_B(T) - \mathbf{1}_{v=B}} d^{m_B(T) + \mathbf{1}_{v=B}}, \end{aligned}$$

where $n_R(T)$ is the number of red vertices in T, $k_B(T)$ is the number of connected components induced by blue vertices, $m_B(T)$ is the number of blue-blue edges, and $\mathbf{1}_{v=B}$ is a characteristic function which takes the value 1 if the color of v is blue and 0 otherwise.

Proof. We are going to show that A and B indeed satisfy (6.5.4) and (6.5.5). Let T be a tree rooted at v and $T_1, \ldots, T_k$ its branches rooted at $v_1, \ldots, v_k$ respectively. Suppose all the vertices except the root are already coloured. We are left with the choice to color v, which can be either red or blue.

- If v is red, then

$$\begin{aligned} n_R(T) &= 1 + \sum_{i=1}^{k} n_R(T_i) \\ k_B(T) &= \sum_{i=1}^{k} k_B(T_i) \\ m_B(T) &= \sum_{i=1}^{k} m_B(T_i), \end{aligned}$$

  Thus, we get a contribution of $a \prod_{i=1}^{k} A(T_i)$ to $A(T)$ and $B(T,v)$.

- If v is blue, then

$$n_R(T) = \sum_{i=1}^{k} n_R(T_i)$$

$$k_B(T) = 1 + \sum_{i=1}^{k} \left(k_B(T_i) - \mathbf{1}_{v_i=B}\right)$$

$$m_B(T) = \sum_{i=1}^{k} (m_B(T_i) + \mathbf{1}_{v_i=B}),$$

These lead to a contribution of $b\prod_{i=1}^{k} B(T_i)$ to $A(T)$ and a contribution of $d\prod_{i=1}^{k} B(T_i)$ to $B(T,v)$.

∎

6.6 Trees with bounded degree sequences

We say that the sequence $A = (a_1, a_2, \ldots, a_n)$ majorizes $B = (b_1, b_2, \ldots, b_n)$ if $a_1 + a_2 + \ldots, a_k \geq b_1 + b_2 + \cdots + b_k$ for all $1 \leq k \leq n$. Then we write $A \triangleright B$. Let us write $D(G)$ for the degree sequence a graph G, $\mathbb{T}_n$ for the set of n-vertex trees, and $\mathbb{S}_n$ for the set of permutations of $1, 2, \ldots, n$. In this section we study the class of graphs

$$\mathbb{T}_B = \{T \in \mathbb{T}_n : B \triangleright D(T)\},$$

for a fixed degree sequence B of a tree. Let ρ be an invariant of rooted trees which satisfies (6.1.1). We say that the tree invariant I is ρ-compatible if for any tree H with fixed leaves v, w, trees $T_1, T_2, \ldots T_r$ with $\rho(T_1) \geq \rho(T_2) \geq \cdots \geq \rho(T_r)$ and $r \geq s \geq r/2$, the maximum value of I among elements of

$$\mathbb{K}_s = \{[T_{\sigma(1)}, \ldots, T_{\sigma(k)}]vHw[T_{\sigma(k+1)}, \ldots, T_{\sigma(r)}] : \sigma \in \mathbb{S}_r \text{ and } r - s \leq k \leq s\}$$

is attained by

$$[T_1, \ldots, T_s]vHw[T_{s+1}, \ldots, T_r] \text{ or } [T_1, \ldots, T_s]wHv[T_{s+1}, \ldots, T_r].$$

In other words, among all possibilities to attach $T_1, T_2, \ldots, T_r$ to v or w in such a way that their degrees are not greater than some bound $s+1$, the maximum value of I is reached when one of v and w has degree $s+1$ for receiving the s T_i's with largest ρ.

Note that if $s \leq s'$ then $\mathbb{K}_s \subseteq \mathbb{K}_{s'}$.

Theorem 6.6.1. *Let I be a ρ-compatible tree invariant, for some ρ that satisfies* (6.1.1)*, and let B be a degree sequence of a tree. Then*

i) $\max\{I(T) : T \in \mathbb{T}_B\} = I(G(B))$ *if f_ρ is increasing,*

ii) $\max\{I(T) : T \in \mathbb{T}_B\} = I(\mathcal{M}(B))$ *if f_ρ is decreasing.*

Proof. We only prove i), a similar idea can be used to prove ii).

Since I is ρ-compatible, $\max\{I(T) : T \in \mathbb{T}_B\}$ is reached by a ρ-exchange-extremal tree, say E. It is only left to prove that E can be chosen to have degree sequence B. Let $T \in \mathbb{T}_B$ have degree sequence $(d_1, d_2, \dots, d_n) = D \neq B = (b_1, b_2, \dots, b_n)$ (thus $B \rhd D$). For $l = \min\{i : d_i \neq b_i\}$, we have $d_l < b_l$. Let $r = \min\{i : i > l \text{ and } d_i > d_{i+1}\}$ and define $D' = (d'_1, d'_2, \dots, d'_n)$ such that $d_i = d'_i$ for all i, except if $i \in \{l, r\}$ for which we have $d'_l = d_l + 1$ and $d'_r = d_r - 1$. It is easy to see that D' is still a decreasing sequence and $D' \rhd D$. For $k \leq l$ or $k \geq r$ we have

$$\sum_{i=1}^{k} d'_i = \sum_{i=1}^{k} d_i \leq \sum_{i=1}^{k} b_i.$$

For $l < k < r$, it is impossible to have

$$\sum_{i=1}^{k} d_i = \sum_{i=1}^{k} b_i.$$

Since $d_{l+1} = d_{l+2} = \cdots = d_r$ and $b_{l+1} \geq b_{l+2} \geq \cdots \geq b_r$, it would lead to

$d_{l+1} + d_{l+2} + \cdots + d_k = (k-l)d_k > b_{l+1} + b_{l+2} + \cdots + b_k$, and $d_k = d_{k+1} > b_k \geq b_{k+1}$ and thus

$$\sum_{i=1}^{k+1} d_i > \sum_{i=1}^{k+1} b_i,$$

which contradicts $B \rhd D$. Hence, we also have

$$\sum_{i=1}^{k} d'_i = 1 + \sum_{i=1}^{k} d_i \leq \sum_{i=1}^{k} b_i$$

in this case. Therefore, $B \rhd D'$.

Let v_1 and v_2 be vertices in T such that $d(v_1) = d_l \geq d_r = d(v_2)$. Then $T = [T_1, \dots, T_{d_l - 1}]v_1 H v_2 [T_{d_l}, \dots, T_{d_l + d_r - 2}]$, for some H and $T_1, T_2, \dots$

$, T_{d_l+d_r-2}$. Let $\sigma \in \mathbb{S}_{d_l+d_r-2}$ such that $\rho(T_{\sigma(1)}) \geq \rho(T_{\sigma(2)}) \geq \cdots \geq \rho(T_{\sigma(d_l+d_r-2)})$. Then there exists $\alpha \in \mathbb{S}_2$ such that $I(T) \leq I(T')$, where

$$T' = [T_{\sigma(1)}, \ldots, T_{\sigma(d_l-1)}]v_{\alpha(1)}Hv_{\alpha(2)}[T_{\sigma(d_l)}, \ldots, T_{\sigma(d_l+d_r-2)}].$$

T' has degree sequence D'. As long as $B \neq D'$, we iterate the process. It ends with a tree with degree sequence B for which the value of I is at least equal to that of any of the previous trees. ■

Corollary 6.6.2. *Let $\mathbb{A} \subseteq \mathbb{T}_n$ and B a degree sequence of an n-vertex tree, such that for any $T \in \mathbb{A}$ we have $B \triangleright D(T)$ and $G(B)$ (resp. $\mathcal{M}(B)$) is in $\mathbb{A}$. For any ρ-compatible tree invariant I for some ρ satisfying* (6.1.1), $\max\{I(T) : T \in \mathbb{A}\} = I(G(B))$ *(resp. $= I(\mathcal{M}(B))$) if f_ρ is increasing (resp. decreasing).*

For example, if $\mathbb{A} = \mathbb{T}_n$ then $B = (n-1, 1, \ldots, 1)$, if $\mathbb{A}$ is the set of all n-vertex trees with vertex degrees at most d then $B = (d, \ldots, d, r, 1, \ldots, 1)$ for some $1 \leq r \leq d$, if $\mathbb{A}$ is the set of n-vertex trees with at most d leaves then $B = (d, 2, \ldots, 2, 1, \ldots, 1)$.

All invariants discussed as examples in previous sections are in fact ρ-compatible.

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