Analysis of tree spectra

by

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Declaration

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Date: December 2018

Abstract

Analysis of tree spectra

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We study the set of eigenvalues (spectrum) of the adjacency matrix, Laplacian matrix and the distance matrix of trees. In particular, we focus on the distribution of eigenvalues in the spectra of large random trees. The families of random trees considered in this work are simply generated trees and increasing trees.

We prove that attaching several copies (two or more) of a tree H to vertices in a tree T "forces" certain real numbers into the adjacency, Laplacian or distance spectrum of the resulting tree. With this construction of forcing subtrees, we prove that the mean proportion of an eigenvalue α in the spectrum of a large random tree is at least the mean number of occurrences of a specific forcing subtree in the large random tree. This gives us explicit lower bounds on the asymptotic mean multiplicity of eigenvalues for different families of random trees.

We prove that the mean proportion of an eigenvalue α in the spectrum of the adjacency matrix and Laplacian matrix of a large simply generated tree can be obtained by solving a system of functional equations. We provide an algorithm to solve this system numerically for a given eigenvalue. For instance, using this algorithm, we show that on average approximately 1.4%, 2.1%, 2.5% and 3.3% of the spectrum of a large pruned binary tree, labelled rooted tree, plane tree and pruned ternary tree respectively consist of the eigenvalue 1. Further, we provide explicit formulas for computing the mean proportion of the eigenvalue 0 in the spectrum of a large simply generated tree.

We also study the spectra of recursive trees and binary increasing trees. We show that the distribution of the eigenvalue 0 (and other eigenvalues) in these random trees satisfies a central limit theorem. We also compute the mean and variance of the multiplicity of the eigenvalue 0 in the spectrum of a large recursive tree and binary increasing tree.

The final chapter deals with related, but somewhat different questions. Given a rooted tree T with leaves $v_1, v_2, \ldots, v_n$, we define the ancestral matrix $C(T)$ of T to be the $n \times n$ matrix for which the entry in the i-th row, j-th column is the level (distance from the root) of the first common ancestor of v_i and v_j. We study properties of this matrix, in particular regarding its spectrum: we obtain several upper and lower bounds for the eigenvalues in terms of other tree parameters. We also find a combinatorial interpretation for the coefficients of the characteristic polynomial of $C(T)$, and show that for d-ary trees, a specific value of the characteristic polynomial is independent of the precise shape of the tree.

Uittreksel

Analise van boomspektra

("Analysis of tree spectra")

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Ons bestudeer die versameling van eiewaardes (spektrum) van die nodusmatriks, Laplace se matriks en die afstandmatriks van bome. In die besonder fokus ons op die verdeling van eiewaardes in die spektra van groot lukrake bome. Die families van lukrake bome wat in hierdie werk beskou word, is eenvoudig gegenereerde bome en toenemende bome.
Ons bewys dat ons 'n aantal kopieë (twee of meer) van 'n boom H aan noduse van 'n boom T kan aanheg om sekere reële getalle in die spektra van die nodusmatriks, Laplace se matriks en die afstandmatriks van die boom wat ontstaan te "forseer". Met hierdie konstruksie van forserende deelbome bewys ons dat die gemiddelde proporsie van 'n eiewaarde α in die spektrum van 'n groot lukrake boom minstens die gemiddelde aantal kopieë van 'n spesifieke forserende deelboom in die groot lukrake boom is. Dit lewer eksplisiete ondergrense vir die asimptotiese gemiddelde veelvoudigheid van eiewaardes vir verskillende families van lukrake bome.
Ons bewys dat die gemiddelde proporsie van 'n eiewaarde α in die spektrum van die nodusmatriks en Laplace se matriks van 'n groot eenvoudig gegenereerde boom verkry kan word deur 'n stelsel funksionele vergelykings op te los. Ons gee 'n algoritme om hierdie stelsel numeries op te los

vir 'n gegewe eiewaarde. Byvoorbeeld kan ons met behulp van hierdie algoritme wys dat 'n gemiddeld van 1.4%, 2.1%, 2.5% en 3.3% van die spektrum van 'n groot gesnoeide binêre boom, gemerkte wortelboom, vlak boom en gesnoeide ternêre boom onderskeidelik uit die eiewaarde 1 bestaan. Verder gee ons eksplisiete formules vir die berekening van die gemiddelde proporsie van die eiewaarde 0 in die spektrum van 'n groot eenvoudig gegenereerde boom.

Ons bestudeer ook die spektra van rekursiewe bome en binêre toenemende bome. Ons wys dat die verdeling van die eiewaarde 0 (en ander eiewaardes) in hierdie lukrake bome 'n sentrale limietstelling bevredig. Ons bereken ook die gemiddeld en die variansie van die veelvoudigheid van die eiewaarde 0 in die spektrum van 'n groot rekursiewe boom en binêre toenemende boom.

Die laaste hoofstuk handel oor verwante, maar ietwat ander vrae. Gegewe 'n gewortelde boom T met blare $v_1, v_2, \ldots, v_n$, definieer ons die voorouermatriks $C(T)$ van T as die $n \times n$ matriks waarvoor die inskrywing in die i-de ry, j-de kolom die vlak (afstand vanaf die wortel) van die eerste gemene voorouer van v_i en v_j is. Ons bestudeer eienskappe van hierdie matriks, veral ten opsigte van sy spektrum: ons kry verskeie bo- en ondergrense vir die eiewaardes in terme van ander boomparameters. Ons vind ook 'n kombinatoriese interpretasie vir die koëffisiënte van die karakteristieke polinoom van $C(T)$, en toon aan dat vir d-êre bome 'n spesifieke waarde van die karakteristieke polinoom onafhanklik is van die presiese vorm van die boom.

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I would like to say thanks to God for given me everything I needed to complete this thesis.
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To my family, colleagues and friends, I say thank you for your love, support and encouragement. God bless you.

Dedications

To my parents

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Chapter 1

Introduction

Spectral graph theory stems from the study of the set of eigenvalues, called spectrum, of matrices associated with graphs. These matrices include the adjacency, distance, Laplacian and signless Laplacian matrices. The main aim is to reveal the properties of graphs that are characterised by the spectra of these matrices. This has yielded several applications in the field of mathematics, physics, chemistry, biology, economics and computer science (see [10], chapter 9). Another important trend in recent literature is the study of the distribution of eigenvalues in the spectra of large random graphs and trees. One such paper, which motivated this work, is the work of Shankar, Steven and Arnab in [5] where they considered some models of random trees and showed that the distribution of eigenvalues in their adjacency spectra has a well-defined limit. However, the characterisation of these limits was not considered. Further, the limiting behaviour of the Laplacian and distance spectra of random trees are still not known. In this work, we study the distribution of eigenvalues in the adjacency and Laplacian spectra of two models of random trees, namely simply generated trees and increasing trees. The plan of the work is as follows.
In Chapter 2, we present some definitions and preliminary results which will be relevant in other chapters. In the following chapter, we focus on subtrees that force specific real numbers to be in the spectrum of a tree. This idea links the distribution of eigenvalues to that of subtrees in a tree. With this, we will come up with lower bounds for the distribution of eigenvalues in some families of random trees. A consequence of this result is the fact that the mean proportion of an eigenvalue in the spectrum of a large random tree is always strictly positive. It is, therefore, an interesting prob-

lem to find an explicit formula to compute this mean proportion for a given eigenvalue. So in Chapter 4, we focus on the mean proportion of eigenvalues in the adjacency and Laplacian spectra of simply generated trees. Here, we provide methods to compute the mean proportion for any eigenvalue. Specifically, we provide an explicit formula to compute the mean distribution of the eigenvalue 0 in the (adjacency) spectrum of large random simply generated trees. In Chapter 5, we present analogous results to Chapter 4 for increasing trees. Here, we compute the mean and variance of the distribution of the eigenvalue 0 in the spectrum of recursive and binary increasing trees. We also show that the distribution of the eigenvalue 0 (and other eigenvalues) in these random trees satisfies a central limit theorem. The final chapter is a joint work with Eric Andriantiana and Stephan Wagner. In this work, we study the spectral properties of a new matrix associated with rooted trees called the ancestral matrix.

Chapter 2

Some preliminary results and basic notions

2.1 Introduction

In this chapter, we present definitions and some results with respect to the spectra of matrices associated with trees and also introduce the families of random trees relevant to our study.

2.2 Spectra of matrices associated with trees

We first define the matrices whose spectrum are considered in our study.

Definition 2.2.1. *The adjacency matrix $A(T)$ of a tree T is the square matrix with entries $a_{ij} = 1$ if the vertices v_i and v_j are adjacent, and $a_{ij} = 0$ otherwise. For the purpose of clarity, we shall call the set of eigenvalues of the adjacency matrix of a tree T the adjacency spectrum of T.*

Definition 2.2.2. *The Laplacian matrix $L(T)$ of a tree T is defined as $L(T) = \mathcal{D}(T) - A(T)$, where $\mathcal{D}(T)$ is a diagonal matrix with the degrees of the vertices of T as its diagonal entries. The Laplacian spectrum of a tree is the set of eigenvalues of its Laplacian matrix.*

Definition 2.2.3. *The distance matrix $D(T)$ of a tree T a matrix whose ij-th entry is the distance (length of a shortest path) between the vertices v_i and v_j in T. We call its set of eigenvalues the distance spectrum of T.*

It is important to note that these matrices are symmetric and hence have real eigenvalues. An important technique we will employ in this work is to observe the relationship between the spectrum of a tree and that of its subtrees. In this regard, a useful tool is the following well-known theorem which captures the relationship between the spectrum of a symmetric matrix and that of its principal sub-matrices.

Theorem 2.2.4 (Cauchy Interlacing Theorem, [24])**.** *Let A be an $n \times n$ hermitian matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, and B be an $m \times m$ submatrix obtained from A by deleting $n-m$ rows and columns of the same index. Suppose B has eigenvalues $\beta_1 \geq \beta_2 \geq \cdots \geq \beta_m$, then*

$$\lambda_i \geq \beta_i \geq \lambda_{n-m+i}, \quad \textit{for } i = \{1, 2, \ldots, m\}.$$

We also state a formula which will be relevant in the proofs of some theorems in the next chapter.

Definition 2.2.5 (Schur Complement formula)**.** *Let A be a block matrix partitioned as shown below,*

$$A = \begin{pmatrix} B_1 & B_2 \\ B_3 & B_4 \end{pmatrix},$$

where B_1 and B_4 are square matrices. Then the determinant of A is given by

$$\det(A) = \det(B_1)\det(B_4 - B_3 B_1^{-1} B_2). \tag{2.1}$$

Now let us introduce the families of random trees related to our work. Note that we will employ the symbolic method, presented in [17, Part A], to define the generating functions of these families of trees.

2.3 Simply generated trees

The main concept of a simply generated tree, introduced by Meir and Moon [30], is to assign non-negative real numbers, called weights, to the nodes (vertices) of a rooted ordered tree with respect to its out-degree sequence. We recall some definitions and introduce some notations.

A **rooted tree** T is a tree with the property that one of its vertices is identified as its root. In view of this definition, we can group the vertices of a rooted tree based on their distances from the root. In particular, a vertex v is said to be on the i-th level if the distance between v and the root r, denoted by $d(v,r)$, is equal to i. Also, we call the vertices on the $(i+1)$-th level that are adjacent to v its **successors** and the number of such vertices its **out-degree** $d^\star(v)$. Therefore, we call the sequence of out-degrees of all vertices in T the **out-degree** sequence.

We can decompose a rooted tree T as a root node r connected to k rooted trees T_j by the edges $\{(r,v_j)\}$, where v_j is the root of $T_j, 1 \leq j \leq k$. The rooted trees $T_j, 1 \leq j \leq k$, are called **branches** of T. This is depicted in Figure 2.1. It is important to note that any vertex v on the i-th level of T can be viewed as the root of its branch. Now, if we take into account the different possible orderings of the successors of each vertex v in a tree T in the plane then we obtain **plane trees.**

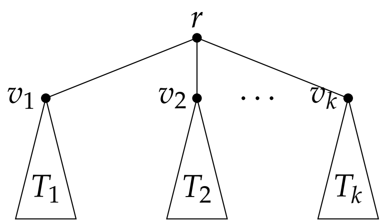


Figure 2.1: The decomposition of a rooted tree T.

Suppose a sequence $(w_k)_{k\geq 0}$ of non-negative real numbers is the weight sequence. Then we define the weight $W(T)$ of a tree T as

$$W(T) = \prod_{v\in V(T)} w_{d^\star(v)} = \prod_{k\geq 0} w_k^{D_k(T)},$$

where $D_k(T)$ is the number of vertices in T with out-degree k. It is easy to see that for a tree T of order n we have

$$\sum_{k\geq 0} D_k(T) = n.$$

We assume that $w_0 > 0$ due to the fact that every tree has a leaf, so setting $w_0 = 0$ would imply $W(T) = 0$ for any tree T.

We define a generating series for the weight sequence by

$$\Phi(t) = \sum_{k\geq 0} w_k t^k.$$

Example 2.3.1. *If we set* $w_k = \frac{1}{k!}$ *for all* $k \geq 0$*, then the weight* $W(T)$ *of the simply generated tree* T *in Figure 2.2 is given by*

$$\begin{aligned} W(T) &= w_0^6 w_1^3 w_2^2 w_4 \\ &= (\frac{1}{0!})^6 (\frac{1}{1!})^3 (\frac{1}{2!})^2 (\frac{1}{4!}) \\ &= \frac{1}{96} \end{aligned}$$

and the generating series for the weight sequence is given by

$$\Phi(t) = \sum_{k \geq 0} \frac{1}{k!} t^k = e^t.$$

We shall see later that these trees with the weight sequence $w_k = \frac{1}{k!}$ *are equivalent to labelled rooted trees.*

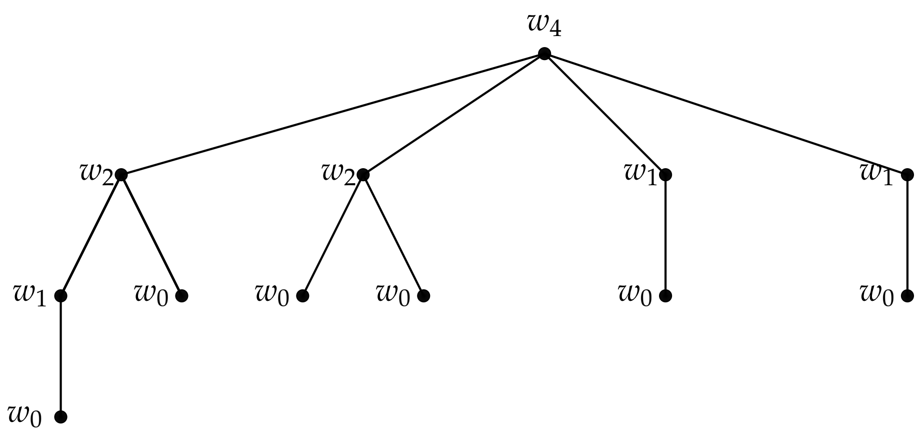


Figure 2.2: A simply generated tree T

Let $\mathbb{T}$ denote the set of all plane (rooted ordered) trees, and let

$$t_n = \sum_{|T|=n} W(T)$$

be the weighted sum of all simply generated trees of order n. We define the generating function $F(x)$, where x marks the size of a tree, to be given by

$$F(x) = \sum_{n \geq 1} t_n x^n = \sum_{T \in \mathbb{T}} W(T) x^{|T|}.$$

Proposition 2.3.2. *[30] The ordinary generating function $F(x)$ of simply generated trees satisfies the equation*

$$F(x) = x\Phi(F(x)) \tag{2.2}$$

Proof. We prove this proposition by considering the decomposition of a tree as indicated earlier and depicted in Figure 2.1. With this, we can write $F(x)$ as

$$\begin{aligned}
F(x) &= \sum_{T\in\mathbb{T}} W(T)x^{|T|} \\
&= \sum_{k\geq 0} w_k \sum_{T_1} \cdots \sum_{T_k} \prod_{j=1}^{k} W(T_j) x^{1+\sum_{j=1}^{k}|T_j|} \\
&= \sum_{k\geq 0} x w_k \prod_{j=1}^{k} \left(\sum_{T_j} W(T_j) x^{|T_j|} \right) \\
&= x \sum_{k\geq 0} w_k F(x)^k \\
&= x\Phi(F(x)).
\end{aligned}$$

∎

Remark 2.3.3. *The implicit equation in Proposition 2.3.2 reveals the weighted recursive structure of simply generated trees. Thus a simply generated tree can be defined as a weighted node or a weighted root joined, by edges, to a collection of simply generated trees. That is,*

$$F(x) = xw_0 + xw_1F(x) + xw_2F(x)^2 + \cdots$$

It is natural to ask where the implicit function (2.2) fails to be analytic, thus, identifying singularities. Actually, this occurs when

$$\frac{\partial}{\partial F(x)} \Big(F(x) - x\Phi(F(x)) \Big) = 0,$$

thus

$$1 - x\Phi'(F(x)) = 0. \tag{2.3}$$

Substituting $x = \frac{F(x)}{\Phi(F(x))}$ from equation (2.2) into equation (2.3) yields

$$\Phi(F(x)) = F(x)\Phi'(F(x)). \tag{2.4}$$

Suppose that equation (2.4) has a positive real solution $F(x) = \tau$, where τ is smaller than the radius of convergence of Φ. If τ exists and the greatest common divisor of $\{k : w_k \neq 0\}$ is equal to 1 ("aperiodicity"), then by Proposition IV.5 in [17, p.278] it is the unique dominant singularity (that is, there is no other singularity with the same or smaller modulus). This means that τ is the smallest, in modulus, with the property that the implicit function theorem fails.

To see this, let us consider the following:

$$\begin{aligned} \tau\Phi'(\tau) - \Phi(\tau) &= 0 \\ \sum_{k\geq 1} kw_k\tau^k - \sum_{k\geq 0} w_k\tau^k &= 0 \\ \sum_{k\geq 1}(k-1)w_k\tau^k &= w_0. \end{aligned}$$

By the triangle inequality we get

$$\left|\sum_{k\geq 1}(k-1)w_k(F(x))^k\right| \leq \sum_{k\geq 1}(k-1)w_k|F(x)|^k \leq \sum_{k\geq 1}(k-1)w_k\tau^k = w_0$$

for $|F(x)| \leq \tau$, and equality holds only if $F(x)^k = \tau^k$ for all k for which $w_k \neq 0$.

Note that τ also corresponds to a singularity ρ with the property that $\tau = F(\rho)$ and

$$\rho = \frac{F(\rho)}{\Phi(F(\rho))} = \frac{\tau}{\tau\Phi'(\tau)} = \frac{1}{\Phi'(\tau)}.$$

With a similar argument one can show that ρ is also the smallest singularity (in modulus) of $F(x)$. Thus

$$|F(x)| = \left|\sum_{n\geq 1} t_n x^n\right| \leq \sum_{n\geq 1} t_n|x|^n \leq \sum_{n\geq 1} t_n\rho^n = \tau$$

for $|x| \leq \rho$ and equality holds only if $x^n = \rho^n$ for all n for which $t_n \neq 0$.

Theorem 2.3.4 ([12], Theorem 3.6)**.** *The ordinary generating function $F(x)$ of simply generated trees satisfies the asymptotic equation*

$$F(x) = \tau - \sqrt{\frac{2\Phi(\tau)}{\Phi''(\tau)}\left(1 - \frac{x}{\rho}\right)} + O\left(\left|1 - \frac{x}{\rho}\right|\right).$$

Proof. Let us consider the Taylor expansion of $\Phi(F(x))$ in equation (2.2) about $F(x) = \tau$. For the sake of simplicity we let $F(x) = \mathcal{F}$. We have

$$\begin{aligned}
\mathcal{F} &= x\left(\Phi(\tau) + \Phi'(\tau)(\mathcal{F}-\tau) + \frac{\Phi''(\tau)(\mathcal{F}-\tau)^2}{2} + \cdots\right)\\
\mathcal{F} - \tau + \tau &= (x-\rho+\rho)\left(\Phi(\tau) + \Phi'(\tau)(\mathcal{F}-\tau) + \frac{\Phi''(\tau)(\mathcal{F}-\tau)^2}{2} + \cdots\right)\\
\mathcal{F} - \tau + \tau &= (x-\rho)\left(\Phi(\tau) + \cdots\right) + \rho\Phi(\tau) + \rho\Phi'(\tau)(\mathcal{F}-\tau)\\
&\quad + \rho\left(\frac{\Phi''(\tau)(\mathcal{F}-\tau)^2}{2} + \cdots\right)
\end{aligned}$$

But we know that $\rho\Phi'(\tau) = 1$ and $\rho\Phi(\tau) = \tau$. So we get

$$\begin{aligned}
\mathcal{F} - \tau + \tau &= (x-\rho)\left(\Phi(\tau) + \cdots\right) + \tau + \mathcal{F} - \tau\\
&\quad + \rho\left(\frac{\Phi''(\tau)(\mathcal{F}-\tau)^2}{2} + \cdots\right)\\
0 &= (x-\rho)\left(\Phi(\tau) + \cdots\right) + \rho\left(\frac{\Phi''(\tau)(\mathcal{F}-\tau)^2}{2} + \cdots\right)\\
-\frac{\rho\Phi''(\tau)(\mathcal{F}-\tau)^2}{2} &= (x-\rho)\left(\Phi(\tau) + \cdots\right) + \rho\left(\frac{\Phi'''(\tau)(\mathcal{F}-\tau)^3}{6} + \cdots\right)\\
(\mathcal{F}-\tau)^2 &= \frac{2}{\Phi''(\tau)}\left(1-\frac{x}{\rho}\right)\left(\Phi(\tau) + \cdots\right)\\
&\quad + \frac{2}{\Phi''(\tau)}\left(\frac{\Phi'''(\tau)(\mathcal{F}-\tau)^3}{6} + \cdots\right)\\
(\mathcal{F}-\tau)^2 &= \frac{2\Phi(\tau)}{\Phi''(\tau)}\left(1-\frac{x}{\rho}\right) + O\left(\left|1-\frac{x}{\rho}\right|^{\frac{3}{2}}\right)\\
\mathcal{F}-\tau &= \pm\sqrt{\frac{2\Phi(\tau)}{\Phi''(\tau)}\left(1-\frac{x}{\rho}\right)\left(1+O\left(\left|1-\frac{x}{\rho}\right|^{\frac{1}{2}}\right)\right)}\\
\mathcal{F}-\tau &= \pm\sqrt{\frac{2\Phi(\tau)}{\Phi''(\tau)}\left(1-\frac{x}{\rho}\right)} + O\left(\left|1-\frac{x}{\rho}\right|\right)\\
\mathcal{F} &= \tau - \sqrt{\frac{2\Phi(\tau)}{\Phi''(\tau)}\left(1-\frac{x}{\rho}\right)} + O\left(\left|1-\frac{x}{\rho}\right|\right). \qquad (2.5)
\end{aligned}$$

The "$-$" sign has to be chosen since $\mathcal{F}$ increases as $x \to \rho^-$.

∎

Now let us introduce some special classes of simply generated trees which we will be relevant to our study.

2.3.1 Plane trees

A plane tree is a rooted tree with the property that the successors of every vertex are arranged by a specified ordering. Due to the earlier mentioned structure of a rooted tree we can view a plane tree as a root r with prescribed ordering of its branches (which are also plane trees). This definition is symbolically represented by

$$\blacktriangle = \bullet \text{ or } \bullet \text{ with sequence}(\blacktriangle).$$

If we let $\mathcal{P}(x)$ be the ordinary generating function of plane trees, where x marks the number of vertices of the tree, then the symbolic definition translates to

$$\begin{aligned}\mathcal{P}(x) &= x + x\mathcal{P}(x) + x\mathcal{P}(x)^2 + x\mathcal{P}(x)^3 + \cdots \\ &= x \sum_{n\geq 0} \mathcal{P}(x)^n \\ &= \frac{x}{1-\mathcal{P}(x)}.\end{aligned} \tag{2.6}$$

In the context of simply generated trees, if we set $w_k = 1$ for $k \geq 0$ we get

$$\Phi(t) = \sum_{k\geq 0} t^k = \frac{1}{1-t},$$

and by Proposition 2.3.2 we obtain the same result as in equation (2.6). Note that with this definition the weight of a plane tree T is always equal to 1.
Now let us consider the implicit equation (2.6) and determine its singularities τ and ρ. We begin by solving equation (2.4) to obtain τ and hence the singularity ρ. Thus

$$\begin{aligned}\Phi(\tau) &= \tau\Phi'(\tau) \\ \frac{1}{1-\tau} &= \frac{\tau}{(1-\tau)^2} \\ 1-\tau &= \tau \\ \tau &= \frac{1}{2}.\end{aligned}$$

Therefore

$$\begin{aligned}\rho &= \frac{1}{\Phi'(\tau)}\\ &= \left(1-\frac{1}{2}\right)^2\\ &= \frac{1}{4}.\end{aligned}$$

By Theorem 2.3.4 we obtain

$$\mathcal{P}(x) = \frac{1}{2} - \sqrt{\frac{1}{4}(1-4x)} + O(|1-4x|).$$

2.3.2 Labelled rooted trees

A **labelled rooted tree** is a rooted tree whereby each vertex is assigned a specific label. Normally, for a tree of order n we assign to each vertex a unique number from the set $\{1, 2, \ldots, n\}$. By considering the earlier mentioned decomposition of a rooted tree, we can view a labelled rooted tree as a labelled node, the root, joined by edges to a set of distinct labelled rooted trees. This is symbolically described by

$$\blacktriangle = \bullet \times \mathsf{Set}\ (\blacktriangle).$$

Let $\mathbb{T}_l$ be the set of all labelled rooted trees. If we let the exponential generating function $L(x)$ be defined as

$$L(x) = \sum_{T\in\mathbb{T}_l} \frac{x^{|T|}}{|T|!}$$

where x marks the sizes of the trees, then from the symbolic definition we get

$$\begin{aligned}L(x) &= \sum_{k\geq 0}\frac{1}{k!}\sum_{T_1}\cdots\sum_{T_k}\binom{|T|-1}{|T_1|,\ldots,|T_k|}|T|\frac{x^{|T|}}{|T|!}\\ &= \sum_{k\geq 0}\frac{1}{k!}\sum_{T_1}\cdots\sum_{T_k}\frac{x^{|T|}}{|T_1|!\cdots|T_k|!}\\ &= x\sum_{k\geq 0}\frac{1}{k!}\left(\sum_{T_1}\frac{x^{|T_1|}}{|T_1|!}\right)\cdots\left(\sum_{T_k}\frac{x^{|T_k|}}{|T_k|!}\right)\\ &= x\sum_{k\geq 0}\frac{1}{k!}L(x)^k\\ &= xe^{L(x)}.\end{aligned}$$

Note that we can obtain the same result if we set the weights w_k of a simply generated tree to be $\frac{1}{k!}$ for all $k \geq 0$ and apply Proposition 2.3.2.
Now, let us consider equation (2.4) and determine the value of the singularity τ and hence ρ. Thus

$$\begin{aligned} e^{\tau} &= \tau e^{\tau} \\ \tau &= 1, \end{aligned}$$

hence

$$\rho = \frac{1}{e}.$$

From Theorem 2.3.4 we get

$$L(x) = 1 - \sqrt{2(1-ex)} + O(|1-ex|).$$

2.3.3 Pruned d-ary trees

A **pruned d-ary tree** is a rooted tree with the property that every vertex has at most d successors. With this definition, we can view a pruned d-ary tree as a root node with $\binom{d}{k}$ possible ways of attaching (by edges) $k \leq d$ pruned d-ary trees, and this is symbolically represented as

$$\blacktriangle = \bullet + \bullet \times \blacktriangle + \binom{d}{2} \bullet \times \blacktriangle^2 + \cdots + \binom{d}{d-1} \bullet \times \blacktriangle^{d-1} + \bullet \times \blacktriangle^d.$$

Suppose we let $\mathbb{T}_d$ be the set of all pruned d-ary trees and $\mathfrak{D}(x)$ their generating function defined as

$$\mathfrak{D}(x) = \sum_{T \in \mathbb{T}_d} x^{|T|}$$

with x marking the sizes of the trees. Then the symbolic definition translates to

$$\begin{aligned} \mathfrak{D}(x) &= x + x\mathfrak{D}(x) + \binom{d}{2} x\mathfrak{D}(x)^2 + \cdots + \binom{d}{d-1} x\mathfrak{D}(x)^{d-1} + x\mathfrak{D}(x)^d \\ &= x(1+\mathfrak{D}(x))^d. \end{aligned} \tag{2.7}$$

One can also derive this formula by setting the weights w_k of simply generated trees to be equal to $\binom{d}{k}$ for all k and applying Proposition 2.3.2. Hence pruned d-ary trees form a class of simply generated trees with $\Phi(t) = (1+t)^d$.

The implicit function (2.7) fails when

$$\begin{aligned}\Phi(\tau) &= \tau\Phi'(\tau)\\(1+\tau)^d &= d\tau(1+\tau)^{d-1}\\1+\tau &= d\tau\\\tau &= \frac{1}{d-1}.\end{aligned}$$

This gives us the singularity

$$\rho = \frac{1}{\Phi'(\tau)} = \frac{(d-1)^{d-1}}{d^d}.$$

Now, let us consider specific cases of pruned d-ary trees whose spectra will be discussed in later sections.

Pruned 2-ary trees are also called **pruned binary trees.** If we let $\mathfrak{D}_2(x)$ be the ordinary generating function for pruned binary trees then by our calculations above $\mathfrak{D}_2(x)$ satisfies the implicit equation

$$\mathfrak{D}_2(x) = x(1+\mathfrak{D}_2(x))^2,$$

which fails to be analytic when $\tau = \mathfrak{D}_2(\rho) = 1$ and $\rho = \frac{1}{4}$.

Similarly, if we set $d = 3$ then such trees are called **pruned ternary trees** with $\mathfrak{D}_3(x)$ as their ordinary generating function satisfying

$$\mathfrak{D}_3(x) = x(1+\mathfrak{D}_3(x))^3,$$

which fails to be analytic when $\tau = \frac{1}{2}$ and $\rho = \frac{4}{27}$.

2.4 Increasing trees

General increasing trees were introduced by Bergeron, Flajolet and Salvy [4] with the idea of assigning weights (non-negative real numbers) to labelled rooted trees, which have the property that labels of nodes increase as one moves along any path from the root to any leaf, based on their outdegree sequence. The generating series $\Phi(t)$ of weights and the weight $W(T)$ of a tree T in a family of increasing trees are defined in a similar way as for simply generated trees.

Example 2.4.1. *Suppose we take the weight sequence to be given by* $(w_k)_{k\geq 0}$, *where* $w_k = \frac{1}{k!}$ *and* k *is the number of outdegree of a node. Then the weight* $W(T)$ *of the increasing tree* T *in Figure 2.3 is given by*

$$\begin{aligned} W(T) &= w_0^6 w_1^3 w_2^2 w_4 \\ &= (\frac{1}{0!})^6 (\frac{1}{1!})^3 (\frac{1}{2!})^2 (\frac{1}{4!}) \\ &= \frac{1}{96}, \end{aligned}$$

and the generating series for the weight sequence is also given by

$$\Phi(t) = \sum_{k\geq 0} \frac{1}{k!} t^k = e^t.$$

We shall see later that this choice of weights yields a family of increasing trees called recursive trees.

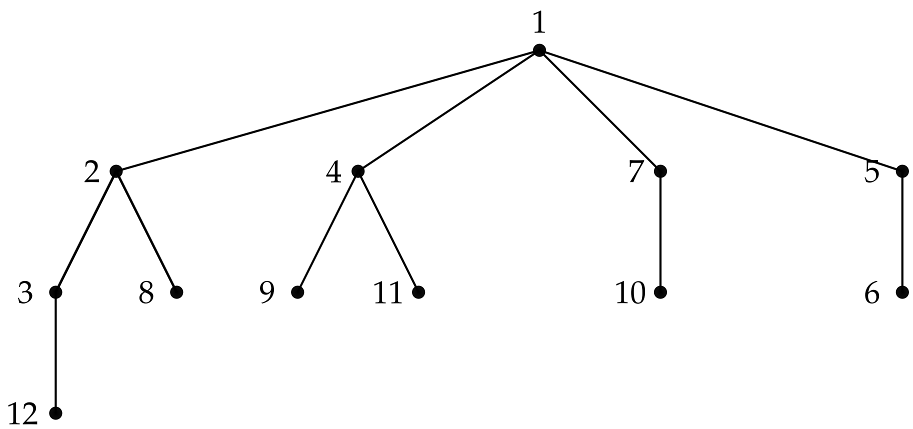


Figure 2.3: An increasing tree T

For a family of increasing trees, we let $\mathcal{T}_n$ be the set of all such trees of order n and $\Phi(t)$ the weight series. We define the exponential generating function for this class of increasing trees as

$$G(x) = \sum_{T\in\mathcal{T}_n} \frac{W(T)x^{|T|}}{|T|!}.$$

It is known [4, Theorem 1] that the generating function $G(x)$ of the family of increasing trees satisfies the differential equation

$$G'(x) = \Phi(G(x)), \quad G(0) = 0.$$

As a result of this characterisation, it is difficult to perform analysis for the general class of increasing trees as opposed to simply generated trees, which satisfies functional equations. Furthermore, Panholzer and Prodinger in [33] showed that there are three families of increasing trees that share a common characterisation, that is they can be obtained by a tree evolution (growth) process. The weight series of these families of increasing trees includes;

1. $\Phi(t) = w_0 e^{\frac{w_1}{w_0}t}$, where $w_0 > 0$ and $w_1 > 0$.
2. $\Phi(t) = w_0 \left(1 - \frac{w_1}{rw_0}t\right)^{-r}$, where $r > 0, w_0 > 0$ and $w_1 > 0$.
3. $\Phi(t) = w_0 \left(1 + \left(\frac{w_1}{dw_0}\right)t\right)^{d}$, where $d > 1, w_0 > 0$ and $w_1 > 0$.

By choosing specific values for w_0, w_1, r and d, we obtain the following families of increasing trees;

1. Recursive trees with weight series $\Phi(t) = e^t$ and $w_0 = w_1 = 1$.
2. Plane oriented recursive trees with weight series $\Phi(t) = \frac{1}{1-t}$ and $w_0 = w_1 = r = 1$.
3. d-ary increasing trees with weight series $\Phi(t) = (1+t)^d, w_0 = 1$ and $w_1 = d$.

In this work, we will focus on solving our main problem for the class of recursive trees and binary increasing trees (2-ary increasing trees).

2.5 Singularity analysis

The main aim of singularity analysis is to extract the asymptotic behaviour of coefficients of meromorphic functions and other complex functions based on their singularities. Flajolet and Sedgewick in [17, Chapter VI] provide analytic transfer theorems that immediately give us the asymptotic behaviour of coefficients of certain functions. In this section, we shall state two such analytic transfer theorems that we will refer to in this work.

Theorem 2.5.1 ([17], p.381). *Suppose $\alpha \in \mathbb{C}\backslash\mathbb{Z}_{\leq 0}$; then for large n, the coefficient of x^n in the power series expansion of*

$$f(x) = (1-x)^{-\alpha}$$

has a full asymptotic expansion in decreasing powers of n as

$$[x^n]f(x) = \frac{n^{\alpha-1}}{\Gamma(\alpha)}\left(1 + \frac{\alpha(\alpha-1)}{2n} + \frac{\alpha(\alpha-1)(\alpha-2)(3\alpha-1)}{24n^2} + \mathcal{O}\Big(\frac{1}{n^3}\Big)\right).$$

Let us consider an analytic transfer theorem that gives us error terms for the coefficients in the expansion of a function from the behaviour near a singularity. Before we state the theorem, we state the following definition.

Definition 2.5.2. *A function $f(x)$ is Δ-analytic if it is analytic in the open domain $\Delta(\phi, R)$ defined as*

$$\Delta(\phi, R) = \{z \Big| |z| < R, z \neq 1, |arg(z-1)| > \phi\}$$

for $R > 1$ and $0 < \phi < \frac{\pi}{2}$.

Theorem 2.5.3 ([17], p.390). *Suppose α and β are arbitrary real numbers and the function $f(x)$ is Δ-analytic.*

1. *Assume that $f(x)$ satisfies in the intersection of a neighbourhood of 1 with its Δ-domain the condition*

$$f(x) = \mathcal{O}\left((1-x)^{-\alpha}\Big(\log\frac{1}{1-x}\Big)^{\beta}\right).$$

Then one has: $[x^n]f(x) = \mathcal{O}(n^{\alpha-1}(\log n)^{\beta})$.

2. *Assume that $f(x)$ satisfies in the intersection of a neighbourhood of 1 with its Δ-domain the condition*

$$f(x) = o\left((1-x)^{-\alpha}\Big(\log\frac{1}{1-x}\Big)^{\beta}\right).$$

Then one has: $[x^n]f(x) = o(n^{\alpha-1}(\log n)^{\beta})$.

From the definition of the above-mentioned families of random trees, it is obvious that they are all rooted trees. With this, let us now focus our attention on the main tree parameter, that is the multiplicity of an eigenvalue in the spectrum a rooted tree.

2.6 Rooted tree classification and additive parameters

In this section, we shall show that the multiplicity of an eigenvalue in the spectrum of a rooted tree can be viewed as an additive parameter and also give a classification of rooted trees based on their spectrum.

We let $N_\alpha(T)$ denote the multiplicity of the eigenvalue α in the spectrum of a rooted tree T. Let $T - r$ be the forest obtained from a rooted tree T by deleting the root r.

Now we let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and $\beta_1 \geq \beta_2 \geq \cdots \geq \beta_{n-1}$ be the eigenvalues of the tree T and the forest $T - r$ respectively. Suppose that $\alpha = \lambda_{k+1}$ has multiplicity l, that is

$$\lambda_1 \geq \cdots \geq \lambda_k > \lambda_{k+1} = \cdots = \lambda_{k+l} > \lambda_{k+l+1} \geq \cdots \geq \lambda_n.$$

Then by the Cauchy Interlacing Theorem (Theorem 2.2.4) we get the following cases;

Case 1:

$$\lambda_k \geq \beta_k > \lambda_{k+1} = \beta_{k+1} = \cdots = \beta_{k+l-1} = \lambda_{k+l} > \beta_{k+l} \geq \lambda_{k+l+1}$$

such that $N_\alpha(T) - N_\alpha(T - r) = l - (l - 1) = 1$,

Case 2:

$$\lambda_k > \beta_k = \lambda_{k+1} = \beta_{k+1} = \cdots = \beta_{k+l-1} = \lambda_{k+l} = \beta_{k+l} > \lambda_{k+l+1}$$

such that $N_\alpha(T) - N_\alpha(T - r) = l - (l + 1) = -1$,

Case 3:

$$\lambda_k > \beta_k = \lambda_{k+1} = \beta_{k+1} = \cdots = \beta_{k+l-1} = \lambda_{k+l} > \beta_{k+l} \geq \lambda_{k+l+1}$$

or

$$\lambda_k \geq \beta_k > \lambda_{k+1} = \beta_{k+1} = \cdots = \beta_{k+l-1} = \lambda_{k+l} = \beta_{k+l} > \lambda_{k+l+1}$$

such that $N_\alpha(T) - N_\alpha(T - r) = l - l = 0$.

This give us an idea of how to classify rooted trees based on their spectrum. To this end, we let $\Psi(T, z)$ and $\Psi_r(T, z)$ be the characteristic polynomials of T and $T - r$ respectively and consider the ratio $\frac{\Psi_r(T,z)}{\Psi(T,z)}$ for a given α. Suppose that the spectrum of T consists of α with multiplicity $N_\alpha(T)$ and p further eigenvalues $\lambda_k, k = \{1, 2, \ldots, p\}$, where $p = n - N_\alpha(T)$. Similarly, suppose the spectrum of $T - r$ consists of α with multiplicity $N_\alpha(T-r)$ and q further eigenvalues $\beta_k, k = \{1, 2, \ldots, q\}$, where $q = n - 1 - N_\alpha(T-r)$. We then get

$$\frac{\Psi_r(T,z)}{\Psi(T,z)} = \frac{(z-\alpha)^{N_\alpha(T-r)} \prod_{k=1}^{q}(z-\beta_k)}{(z-\alpha)^{N_\alpha(T)} \prod_{k=1}^{p}(z-\lambda_k)}. \tag{2.8}$$

With this, we get three types of rooted trees which are defined in the following way.
If $N_\alpha(T) < N_\alpha(T-r)$, then $\frac{\Psi_r(T,z)}{\Psi(T,z)}$ has a zero at $z = \alpha$ and $N_\alpha(T) - N_\alpha(T-r) = -1$, hence T is called a **type zero** tree.
On the other hand, if $N_\alpha(T) > N_\alpha(T-r)$, then $\frac{\Psi_r(T,z)}{\Psi(T,z)}$ has a pole at $z = \alpha$ and $N_\alpha(T) - N_\alpha(T-r) = 1$, hence the tree T is called a **type pole** tree.
Lastly, T is called a **type $\mathcal{C}$** tree if $N_\alpha(T) = N_\alpha(T-r)$ and $\frac{\Psi_r(T,z)}{\Psi(T,z)}$ has a non-zero value in the limit as z approaches α. Another important property that we need to check is the sign of the limit, and to do so we consider angles of a tree.
Let $A(T)$ be the adjacency matrix of a tree T of order n with distinct eigenvalues $\lambda_1, \lambda_2, \ldots \lambda_m$, where $m \leq n$. For an eigenvalue λ_i, we let $\xi(\lambda_i)$ be its **eigenspace** and $\boldsymbol{y}_j, 1 \leq j \leq k$, an orthonormal basis of its eigenspace (which are also eigenvectors corresponding to λ_i). Now, if we define $P_i, 1 \leq i \leq m$, to be the matrix of the form

$$P_i = \boldsymbol{y}_1\boldsymbol{y}_1^T + \boldsymbol{y}_2\boldsymbol{y}_2^T + \cdots + \boldsymbol{y}_k\boldsymbol{y}_k^T,$$

then we get

$$A(T) = \sum_{i=1}^{m} \lambda_i P_i.$$

Suppose $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_n\}$ are the natural basis of $\mathbb{R}^n$. Then the values of $\theta_{ij} = ||P_i e_j||, 1 \leq i \leq m$ and $1 \leq j \leq n$, are called the **angles of the tree** T. The following theorem provides information about the relation between the angles of T and $\frac{\Psi_r(T,z)}{\Psi(T,z)}$.

Theorem 2.6.1 ([10], p. 33)**.** *Let $\Psi(T,z)$ and $\Psi_r(T,z)$ be the characteristic polynomials of a tree T and the forest $T-r$ respectively. Suppose $\lambda_1, \lambda_2, \ldots \lambda_m$ are the distinct eigenvalues of T and θ_{ij} are its angles. Then*

$$\frac{\Psi_r(T,z)}{\Psi(T,z)} = \sum_{i=1}^{m} \frac{\theta_{ir}^2}{z-\lambda_i},$$

where $\theta_{ir} = ||P_i \boldsymbol{e}_r||$ *and* $\boldsymbol{e}_r$ *is the natural basis vector of* $\mathbb{R}^n$ *with respect to the root* r.

From Theorem 2.6.1 we have that

$$\begin{aligned}
\lim_{z\to\lambda_k}(z-\lambda_k)\frac{\Psi_r(T,z)}{\Psi(T,z)} &= \lim_{z\to\lambda_k}(z-\lambda_k)\sum_{i=1}^{m}\frac{\theta_{ir}^2}{z-\lambda_i} \\
&= \lim_{z\to\lambda_k}\theta_{kr}^2 + (z-\lambda_k)\sum_{i\neq k}^{m}\frac{\theta_{ir}^2}{z-\lambda_i} \\
&= \theta_{kr}^2 \\
&\geq 0.
\end{aligned}$$

This shows that the limit is always non-negative. In particular, the limit θ_{kr}^2 is positive when $\frac{\Psi_r(T,z)}{\Psi(T,z)}$ has a pole at $z = \lambda_k$ and 0 otherwise. Another important key feature of the ratio $\frac{\Psi_r(T,z)}{\Psi(T,z)}$ is captured in the following theorem.

Theorem 2.6.2 ([31]). *Let* $\Psi(T,z)$ *and* $\Psi_r(T,z)$ *be the characteristic polynomials of a tree* T *and the forest* $T-r$ *respectively, where* r *is the root of* T*. Suppose* $T_1, T_2, \ldots, T_k$ *are the branches of* T *with* $v_1, v_2, \ldots, v_k$ *their respective roots. Then*

$$\frac{\Psi_r(T,z)}{\Psi(T,z)} = \frac{1}{z - \sum_{j=1}^{k}\frac{\Psi_{v_j}(T_j,z)}{\Psi(T_j,z)}}. \tag{2.9}$$

An immediate consequence of Theorem 2.6.2 is the following result that characterises a type zero tree.

Theorem 2.6.3. *A rooted tree* T *is a type zero tree if and only if at least one of the branches is a type pole tree.*

Proof. Let T be a type zero rooted tree. Then we know that $\frac{\Psi_r(T,z)}{\Psi(T,z)}$ has a zero at $z = \alpha$. By equation (2.9), this implies that there is at least one branch T_j such that $\frac{\Psi_{v_j}(T_j,\alpha)}{\Psi(T_j,\alpha)} = \infty$. It then follows that T has at least one type pole branch.

Conversely, suppose that at least one of the branches of T is a type pole branch (that is, for such a branch T_j, $\frac{\Psi_{v_j}(T_j,z)}{\Psi(T_j,z)}$ has a pole at $z = \alpha$). We need to show that the poles in the summand $\sum_{j=1}^{k}\frac{\Psi_{v_j}(T_j,z)}{\Psi(T_j,z)}$ do not cancel out. From Theorem 2.6.1, we deduce that for any eigenvalue λ_k of T,

$$\lim_{z\to\lambda_k}(z-\lambda_k)\frac{\Psi_r(T,z)}{\Psi(T,z)} \geq 0.$$

This implies that the sign is always the same (i.e., positive) for each summand in $\sum_{j=1}^{k} \frac{\Psi_{v_j}(T_j,z)}{\Psi(T_j,z)}$ as $z \to \alpha$. In particular, if we let c_j be the number of distinct eigenvalues of T_j and also $\theta_{iv_j} = ||P_i \boldsymbol{e}_{v_j}||$, where $\boldsymbol{e}_{v_j}$ is the natural basis vector of $\mathbb{R}^{|T_j|}$ corresponding to the root v_j, then we get

$$\begin{aligned}\lim_{z\to\lambda_l}(z-\lambda_l)\sum_{j=1}^{k}\frac{\Psi_{v_j}(T_j,z)}{\Psi(T_j,z)} &= \lim_{z\to\lambda_l}\sum_{j=1}^{k}(z-\lambda_l)\sum_{i=1}^{c_j}\frac{\theta_{iv_j}^2}{z-\lambda_i}\\ &= \sum_{j=1}^{k}\theta_{lv_j}^2\\ &> 0.\end{aligned}$$

Since the poles do not cancel out, we obtain from equation (2.9) that

$$\lim_{z\to\alpha}\frac{\Psi_{v_j}(T,z)}{\Psi(T,z)} = 0.$$

Hence T is a type zero tree. This completes the proof.

■

Suppose we define $S(z)$ by

$$S(z) = \sum_{j=1}^{k}\frac{\Psi_{v_j}(T_j,z)}{\Psi(T_j,z)}.$$

Then it is clear that if $S(\alpha) = \alpha$, $\frac{\Psi_r(T,z)}{\Psi(T,z)}$ has a pole at $z = \alpha$ and hence T is a type pole rooted tree, otherwise it is a type $\mathcal{C}$ tree if none of its branches is a type pole.

Remark 2.6.4. *It can be observed that the Cauchy Interlacing Theorem (Theorem2.2.4) is the key theorem in the approach of classifying rooted trees based on their spectrum. In order to extend this result to the Laplacian spectrum of rooted trees, we consider planted rooted trees, which are rooted trees with a hidden vertex attached to the root. With this, the degree of the root increases by 1. The Laplacian matrix of the planted rooted tree then satisfies the interlacing theorem and hence gives us the same rooted tree classification based on the Laplacian spectrum. Further, the difference between the multiplicity of an eigenvalue α in the Laplacian spectrum of a rooted tree T and that of the corresponding planted rooted T^* is at most 1 since their Laplacian matrices only differ in one entry (corresponding to the root). It thus* *suffices to study the spectrum of large planted rooted trees. Due to the fact that the distance spectrum does not satisfy the interlacing theorem by this construction, our method is not sufficient to study the distance spectrum.*

Based on the classification of rooted trees, we can now define $N_\alpha(T)$ as an additive parameter. Let T be a rooted tree with root r and k branches $T_j, 1 \leq j \leq k$. We treat the multiplicity of eigenvalue α in the spectrum or Laplacian spectrum of a large rooted tree T, denoted by $N_\alpha(T)$, as an additive parameter satisfying the recursion

$$N_\alpha(T) = \sum_{i=1}^{k} N_\alpha(T_i) + n_\alpha(T),$$

where the toll function $n_\alpha(T)$ is given by

$$n_\alpha(T) = N_\alpha(T) - N_\alpha(T - r).$$

Chapter 3

Forcing subtrees

3.1 Introduction

In this chapter, we are interested in the distribution of eigenvalues in the spectrum of the adjacency matrix, Laplacian matrix and the distance matrix of a tree. The main objective of this chapter is motivated by the results captured in the following theorem.

Theorem 3.1.1 ([7]). *Let $\mathcal{T}_n$ be the set of labelled trees of order n and H a given finite tree. Then the limiting distribution of the number of occurrences of H (as induced subtrees) in a tree of $\mathcal{T}_n$ is asymptotically normal with mean asymptotically equivalent to μn, where $\mu > 0$ depends on the pattern H.*

The main idea is as follows: suppose there exists a pattern formed by subtrees that “forces" certain real numbers to be in the spectrum of a tree. Then by Theorem 3.1.1 we know that for every “forced" real number α, there exists a positive constant c_α such that α will occur at least $c_\alpha n$ times on average in the spectrum of a large labelled random tree with n vertices. Therefore, our main objective is to identify the relationship between the spectrum of subtrees in a tree T and the spectrum of T. The families of random trees that we shall consider in this work are simply generated trees and increasing trees. The distribution of graph parameters in these families of random trees have received considerable attention. Among these is the average number of occurrences of a subtree (a node with its descendants) in random trees. It is known [2, 15, 18, 27, 38] that the mean proportion is strictly positive and every possible subtree occurs with high probability. We provide some definitions and notations which will be relevant to our study.

We can decompose a rooted tree T as a root node r connected to k rooted trees T_j (branches) by the edges $\{(r, v_j)\}$, where v_j is the root of T_j, $1 \leq j \leq k$. By this, we can also treat the number of occurrences of a subtree S in a tree T, denoted by $\mathcal{N}_S(T)$, as an additive parameter satisfying the recursion

$$\mathcal{N}_S(T) = \sum_{i=1}^{k} \mathcal{N}_S(T_i) + n_S(T),$$

where the toll function $n_S(T)$ is given by

$$n_S(T) = \begin{cases} 1 & \text{if } T = S, \\ 0 & \text{otherwise.} \end{cases}$$

For a tree T, we let $V(T)$ and $E(T)$ denote the set of its vertices and edges respectively. Suppose G and H are two trees (not necessarily distinct), we let $G \uplus H$ denote their disjoint union. Also, we let $G_u \circ H_v$ denote a tree obtained from G and H by joining a vertex $u \in V(G)$ to a vertex $v \in V(H)$ by the edge uv. This is depicted in Figure 3.1. Further, if we join k (where $k \geq 2$) copies of H to the same vertex u in G then the resulting tree is denoted by $G_u \circ H_v^k$.

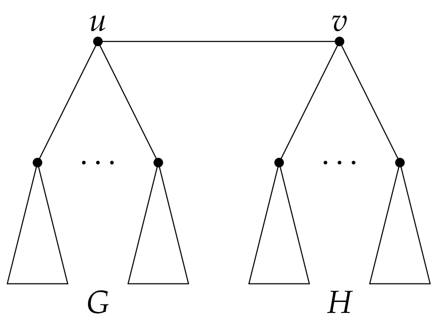


Figure 3.1: A tree $G_u \circ H_v$.

Now let us focus on the spectrum of the above-mentioned matrices associated to trees. For each case, we shall present a relationship between the spectrum of a tree and that of its subtrees. It is important to note that for an empty tree T (tree with no vertices) we set its characteristic polynomial to be equal to 1.

3.2 Adjacency spectrum

In this section, we study the adjacency spectrum, which is the set of eigenvalues of the adjacency matrix, of trees. We begin with the following results on the characteristic polynomial of a simple graph $G \uplus H$ and that of its components G and H.

Theorem 3.2.1 ([10], p.25)**.** *Suppose $\Psi_G(x)$ and $\Psi_H(x)$ are the characteristic polynomials of the adjacency matrices of the graphs G and H respectively. Then the characteristic polynomial of the adjacency matrix of $G \uplus H$ is given by*

$$\Psi_{G\uplus H}(x) = \Psi_G(x)\Psi_H(x).$$

Proof. Let O be a matrix with all entries equal to zero. Also, we let $A(G)$ and $A(H)$ be the adjacency matrices of G and H respectively. Then we get

$$A(G \uplus H) = \begin{pmatrix} A(G) & O \\ O & A(H) \end{pmatrix}.$$

Therefore, the characteristic polynomial of $A(G \uplus H)$ is given by

$$\begin{aligned} \Psi_{G\uplus H}(x) &= Ix - A(G \uplus H) \\ &= \begin{vmatrix} Ix - A(G) & O \\ O & Ix - A(H) \end{vmatrix}. \end{aligned}$$

Using equation (2.1), we get

$$\begin{aligned} \Psi_{G\uplus H}(x) &= \det(Ix - A(G)) \det(Ix - A(H)) \\ &= \Psi_G(x)\Psi_H(x). \end{aligned}$$

■

Remark 3.2.2. *It follows directly from Theorem 3.2.1 that the spectrum of $G \uplus H$ is equal to the union of the spectra of its components G and H. Further, it is important to note that an analogous statement of Theorem 3.2.1 can also be made for the Laplacian matrix $L(G \uplus H)$ and the signless Laplacian matrix $S(G \uplus H)$ of the simple graph $G \uplus H$.*

A simple graph whose connected components are all trees is called a forest.

Corollary 3.2.3. *The spectrum of a forest contains the spectrum of all the connected components.*

Proof. Let F be a forest consisting of k trees $T_1, T_2, \ldots, T_k$. We can write $F = T_1 \uplus T_2 \uplus \cdots \uplus T_k$ and the result follows immediately from Theorem 3.2.1. ∎

When we join k_i copies of H to different vertices $u_i, i = \{1, 2, \ldots, l\}$ in a tree T, we can bound the multiplicities of certain eigenvalues in the resulting tree from below. This is captured in the following results.

Theorem 3.2.4. *Let T be a tree obtained from G by joining k_i copies of the tree H to the vertices $u_i \in V(G), i = \{1, 2, \ldots, l\}$. Then each eigenvalue of H is an eigenvalue of the resulting tree, and the multiplicity of each of these "forced" eigenvalues is at least $\sum_{i=1}^{l}(k_i - 1)$.*

Proof. Consider the forest $T \backslash \{u_1, u_2, \ldots, u_l\}$. Obviously, it has $k_1 + k_2 + \cdots + k_l$ components isomorphic to H. So if α is an eigenvalue of H, then it is an eigenvalue of $T \backslash \{u_1, u_2, \ldots, u_l\}$ whose multiplicity is at least $k_1 + k_2 + \cdots + k_l$. Therefore, the interlacing theorem shows that the multiplicity of α as an eigenvalue of T differs from the multiplicity as an eigenvalue of $T \backslash \{u_1, u_2, \ldots, u_l\}$ by at most l. Thus, α is an eigenvalue of T with multiplicities at least

$$k_1 + k_2 + \cdots + k_l - l = (k_1 - 1) + (k_2 - 1) + \cdots + (k_l - 1).$$

∎

Let $l(T)$ be the number of leaves in the tree T. Also, let $q(T)$ be the number of quasipendant vertices (those vertices adjacent to the leaves) in the tree T.

Corollary 3.2.5 ([32],[36],[9] p.258)**.** *The multiplicity of the eigenvalue zero in the adjacency spectrum of a tree T is at least $l(T) - q(T)$.*

Proof. Let the quasipendant vertices in T be $v_1, v_2, \ldots, v_m$ such that the respective number of leaves attached to them are $l_1, l_2, \ldots, l_m$. Let K_1 be the complete graph of order one. We know that the l_1 leaves attached to v_1 are equivalent to l_1 copies of K_1 joined to v_1. We know that 0 is an eigenvalue of K_1. Therefore, by Theorem 3.2.4, the multiplicity of the eigenvalue 0 is at least

$$\sum_{i=1}^{m}(l_i - 1) = \sum_{i=1}^{m} l_i - m = l(T) - q(T).$$

∎

3.3 Laplacian spectrum

In this section, we study the Laplacian spectrum of trees. It is known that the Laplacian and the signless Laplacian spectrum of a tree are the same. In view of that, we shall only consider the Laplacian spectrum for trees and remark that analogous results also hold for the signless Laplacian spectra of simple graphs (in general). We first provide some definitions and explain some notations (which we will use for the sake of simplicity).

For a vertex v in a graph G we denote the set of its neighbours and the cardinality of that set (called its degree) by $N(v)$ and d_v respectively.

Suppose that $V^\star$ is a subset of the set of vertices $V(G)$ of a tree G. Then we let $L(G)_{V^\star}$ be a submatrix obtained from $L(G)$ by deleting the rows and columns (of the same index) associated to the vertices in $V^\star$. If $V^\star = \{u\}$, then we write $L(G)_u$ instead. Also, we let $L^r(G : V^\star)$ denote a matrix obtained from $L(G)$ by adding $r \in \mathbb{N}$ to the degrees (diagonal entries) of the vertices in $V^\star$. In particular, we obtain $L^r(G : u)$ from $L(G_u \circ H_v^r)$ by deleting all the rows and columns (of the same index) associated to the vertices of the r copies of H.

Proposition 3.3.1. *Let $L^r(G : u)$ be a matrix obtained from $L(G)$ by adding $r \in \mathbb{N}$ to the degree of a vertex u in G. Then the characteristic polynomial of $L^r(G : u)$ is given by*

$$\Psi_{L^r(G:u)}(x) = \Psi_{L(G)}(x) - r\Psi_{L(G)_u}(x).$$

Proof. From the definition of $L^r(G)$ we get

$$L^r(G : u) = \begin{pmatrix} L(G)_u & -\boldsymbol{r} \\ -\boldsymbol{r}^T & d_u + r \end{pmatrix},$$

where the i-th entry of $\boldsymbol{r}$ is

$$r_i = \begin{cases} 1 & \text{if } iu \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

Therefore,

$$\begin{aligned} \Psi_{L^r(G:u)}(x) &= \begin{vmatrix} Ix - L(G)_u & \boldsymbol{r} \\ \boldsymbol{r}^T & x - d_u - r \end{vmatrix} \\ &= \begin{vmatrix} Ix - L(G)_u & \boldsymbol{r} \\ \boldsymbol{r}^T & x - d_u \end{vmatrix} + \begin{vmatrix} Ix - L(G)_u & \boldsymbol{r} \\ \mathbf{0}^T & -r \end{vmatrix} \\ &= \Psi_{L(G)}(x) - r\Psi_{L(G)_u}(x). \end{aligned}$$

■

Theorem 3.3.2 ([23], Lemma 8)**.** *The characteristic polynomial of $L(G_u \circ H_v)$ is given by*

$$\Psi_{L(G_u \circ H_v)}(x) = \Psi_{L^1(H:v)}(x)\Psi_{L^1(G:u)}(x) - \Psi_{L(G)_u}(x)\Psi_{L(H)_v}(x).$$

Proof. We can write $A(G_u \circ H_v)$ as

$$A(G_u \circ H_v) = \begin{pmatrix} G^\star & \boldsymbol{r} & \mathbf{0} & O \\ \boldsymbol{r}^T & 0 & 1 & \mathbf{0}^T \\ \mathbf{0}^T & 1 & 0 & \boldsymbol{s}^T \\ O^T & \mathbf{0} & \boldsymbol{s} & H^\star \end{pmatrix},$$

where $G^\star = A(G-u), H^\star = A(H-v)$ and $\mathbf{0}$ is a vector with all entries equal to zero. Also, the i-th entries of $\boldsymbol{r}$ and $\boldsymbol{s}$ are

$$r_i = \begin{cases} 1 & \text{if } iu \in E(G), \\ 0 & \text{otherwise,} \end{cases} \quad \text{and} \quad s_i = \begin{cases} 1 & \text{if } iv \in E(H), \\ 0 & \text{otherwise.} \end{cases}$$

respectively.
Therefore, we get the characteristic polynomial of $L(G_u \circ H_v)$ to be given by

$$\begin{aligned} \Psi_{L(G_u \circ H_v)}(x) &= \begin{vmatrix} Ix - L(G)_u & \boldsymbol{r} & \mathbf{0} & O \\ \boldsymbol{r}^T & x - d_u - 1 & 1 & \mathbf{0}^T \\ \mathbf{0}^T & 1 & x - d_v - 1 & \boldsymbol{s}^T \\ O & \mathbf{0} & -\boldsymbol{s} & Ix - L(H)_v \end{vmatrix} \\ &= \begin{vmatrix} Ix - L(G)_u & \boldsymbol{r} & \mathbf{0} & O \\ \boldsymbol{r}^T & x - d_u - 1 & 1 & \mathbf{0}^T \\ \mathbf{0}^T & 0 & x - d_v - 1 & \boldsymbol{s}^T \\ O & \mathbf{0} & -\boldsymbol{s} & Ix - L(H)_v \end{vmatrix} \\ &\quad + \begin{vmatrix} Ix - L(G)_u & \boldsymbol{r} & \mathbf{0} & O \\ \boldsymbol{r}^T & x - d_u - 1 & 1 & \mathbf{0}^T \\ \mathbf{0}^T & 1 & 0 & \mathbf{0}^T \\ O & \mathbf{0} & -\boldsymbol{s} & Ix - L(H)_v \end{vmatrix}. \end{aligned}$$

Using the Schur complement formula, equation (2.1), we get

$$
\begin{aligned}
\Psi_{L(G_u \circ H_v)}(x) = &\begin{vmatrix} Ix - L(G)_u & \boldsymbol{r} \\ \boldsymbol{r}^T & x - d_u - 1 \end{vmatrix} \begin{vmatrix} x - d_v - 1 & \boldsymbol{s}^T \\ \boldsymbol{s} & Ix - L(H)_v \end{vmatrix} \\
&- \det(Ix - L(H)_v) \begin{vmatrix} Ix - L(G)_u & \mathbf{0} \\ \boldsymbol{r}^T & 1 \end{vmatrix} \\
&= \Psi_{L^1(H:v)}(x)\Psi_{L^1(G:u)}(x) - \Psi_{L(G)_u}(x)\Psi_{L(H)_v}(x).
\end{aligned}
$$

■

Note that we can rewrite $L(G)_u$ and $L(H)_v$ as $L^1(G-u : N(u))$ and $L^1(H - v : N(v))$ respectively.
As for the adjacency spectrum, attaching copies of a fixed tree H in different places "forces" certain eigenvalues to be part of the spectrum of the resulting tree. We also study the multiplicities of the "forced" eigenvalues in the Laplacian spectrum when several copies of a tree H are attached to different vertices of a tree G. This is captured in the following theorem.

Theorem 3.3.3. *Let T be a tree obtained from G by joining k_i copies of the tree H, each at the same vertex v of H, to the vertices $v_i \in V(G)$, $i = \{1, 2, \ldots, l\}$. Then the multiplicity of each eigenvalue of $L^1(H : v)$ in the Laplacian spectrum of T is at least $\sum_{i=1}^{l}(k_i - 1)$.*

Proof. The proof is similar to the proof of Theorem 3.2.4. Let T be a tree obtained from G by joining k_i copies of the tree H, each at the same vertex v of H, to the vertices $v_i \in V(G)$, $i = \{1, 2, \ldots, l\}$. Let $T^\star$ be a forest consisting of $k_1 + k_2 + \cdots + k_l$ copies of H. If we delete rows and columns of $L(T)$ corresponding to vertices in G then we get $L^1(T^\star : v)$ as a principal submatrix of $L(T)$. Suppose α is an eigenvalue of $L^1(H : v)$. Then we know that it is also an eigenvalue of $L^1(T^\star : v)$ with multiplicity at least $k_1 + k_2 + \cdots + k_l$. By the interlacing theorem, the difference between the multiplicity of α as an eigenvalue of $L^1(T^\star : v)$ and that of $L(T)$ is at most l. Hence we get the required result.

■

Corollary 3.3.4 ([14, 22])**.** *The multiplicity of the eigenvalue 1 in the Laplacian spectrum of a tree T is at least $l(T) - q(T)$.*

Proof. The proof is analogous to that of Corollary 3.2.5 by considering the fact that the matrix $L^1(K_1 : v)$ is the matrix $[1]$, whose only eigenvalue is 1. ∎

Remark 3.3.5. *It is important to note that these results also hold when considering the signless Laplacian spectrum of simple graphs. Futher, it can be deduced from the above results that we can always force any real number that occurs as an eigenvalue of the matrix $L^1(T : u)$, for u in the vertex set of a tree T, to be in the Laplacian spectrum of another tree $T^\star$ by the above construction. Unlike the adjacency spectrum of trees, we cannot force all real numbers that occur in the Laplacian spectrum of trees in this way. For instance, it is well known that the multiplicity of the eigenvalue 0 in the Laplacian spectrum of a graph is equal to the number of connected components. Now, since all trees are connected, the multiplicity of the eigenvalue 0 is always 1. Also, Robert, Russell and Sunder in [22] showed that for any positive integer $\lambda > 1$, the multiplicity of λ as an eigenvalue of $L(T)$ of any tree T is equal to 1. This implies that, we cannot force positive integer eigenvalues greater than 1. It follows immediately that the matrix $L^1(T : u)$ of a tree T is positive definite and does not contain any positive integer greater than one. Moreover, the spectrum of $L^1(T : u)$ varies when a different vertex $v \neq u$ in T is used for the construction.*

3.4 Distance spectrum

In this section, we study the distance spectrum of trees. We shall provide some definitions and notations that will be relevant to our work.

Let $\mathbf{1}$ and J denote the vector and the matrix respectively whose entries are all one.

Let $D(T)$ denote the distance matrix of a tree T. Let $\boldsymbol{r}$ be the column in $D(T)$ as associated with the vertex $v \in V(T)$. Let $\mathbb{D}_v(T)$ be a matrix obtained from $D(T)$ by subtracting $\boldsymbol{r} + \mathbf{1}$ from all the rows and columns of $D(T)$. For simplicity, we say $\mathbb{D}_v(T)$ is constructed with respect to the vertex v. We have,

$$\begin{aligned}\mathbb{D}_v(T) &= D(T) - [\mathbf{1}(\boldsymbol{r}+\mathbf{1})^T + (\boldsymbol{r}+\mathbf{1})\mathbf{1}^T] \\ &= D(T) - [\mathbf{1}\boldsymbol{r}^T + \boldsymbol{r}\mathbf{1}^T + 2J].\end{aligned}$$

We set $R_v(T) = \mathbf{1}\boldsymbol{r}^T + \boldsymbol{r}\mathbf{1}^T + 2J$ to get $\mathbb{D}_v(T) = D(T) - R_v(T)$.

The following result captures the relationship between the spectrum of $\mathbb{D}_v(T)$ and the distance spectrum of $G_u \circ T_v^2$.

Theorem 3.4.1. *Let G and T be any two trees. The distance spectrum of the tree $G_u \circ T_v^2$ contains the spectrum of $\mathbb{D}_v(T)$.*

Proof. Let $\boldsymbol{s}$ and $\boldsymbol{r}$ be the columns in $D(G)$ and $D(T)$ corresponding to the vertices u and v respectively. We can write the distance matrix of the tree $G_u \circ T_v^2$ as follows;

$$D(G_u \circ T_v^2) = \begin{pmatrix} D(G) & Q & Q \\ Q^T & D(T) & R_v(T) \\ Q^T & R_v(T) & D(T) \end{pmatrix},$$

where $Q = (\boldsymbol{s} + \mathbf{1})\mathbf{1}^T + \mathbf{1}^T \boldsymbol{r}$.

Let $\boldsymbol{x}$ be an eigenvector corresponding to eigenvalue λ of the matrix $\mathbb{D}_v(T)$. If we consider the vector $\boldsymbol{y} = (\mathbf{0}, \boldsymbol{x}, -\boldsymbol{x})^T$, we get

$$\begin{aligned} D(G_u \circ T_v^2)\boldsymbol{y} &= \begin{pmatrix} D(G) & Q & Q \\ Q^T & D(T) & R_v(T) \\ Q^T & R_v(T) & D(T) \end{pmatrix} \begin{pmatrix} \mathbf{0} \\ \boldsymbol{x} \\ -\boldsymbol{x} \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{0} \\ (D(T) - R_v(T))\boldsymbol{x} \\ -(D(T) - R_v(T))\boldsymbol{x} \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{0} \\ (\mathbb{D}_v(T))\boldsymbol{x} \\ -(\mathbb{D}_v(T))\boldsymbol{x} \end{pmatrix} \\ &= \lambda \boldsymbol{y}. \end{aligned}$$

This implies that λ is also an eigenvalue of $D(G_u \circ T_v^2)$ corresponding to the eigenvector $\boldsymbol{y}$. This completes the proof. ∎

This leads to the following results.

Theorem 3.4.2. *Let G and T be any two trees. The distance spectrum of the tree $G_u \circ T_v^k$ contains the spectrum of $\mathbb{D}_v(T)$ with multiplicity at least $k-1$.*

Proof. The distance matrix of $D(G_u \circ T_v^k)$ is given by

$$D(G_u \circ T_v^k) = \begin{pmatrix} D(G) & Q & Q & \cdots & Q \\ Q^T & D(T) & R_v(T) & \cdots & R_v(T) \\ Q^T & R_v(T) & D(T) & \ddots & R_v(T) \\ \vdots & \vdots & \ddots & \ddots & R_v(T) \\ Q^T & R_v(T) & \cdots & R_v(T) & D(T) \end{pmatrix}.$$

Let $\boldsymbol{x}$ be an eigenvector corresponding to eigenvalue λ of the matrix $\mathbb{D}_v(T)$. Let Y be the $n \times (k-1)$ matrix defined as

$$Y = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \boldsymbol{x} & \boldsymbol{x} & \boldsymbol{x} & \cdots & \boldsymbol{x} \\ -\boldsymbol{x} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & -\boldsymbol{x} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -\boldsymbol{x} & \cdots & \mathbf{0} \\ \vdots & \ddots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & -\boldsymbol{x} \end{pmatrix}.$$

Here, n is the order of $G_u \circ T_v^k$. Now if we compute $D(G_u \circ T_v^k)Y$ we get

$$D(G_u \circ T_v^k)Y = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \lambda\boldsymbol{x} & \lambda\boldsymbol{x} & \lambda\boldsymbol{x} & \cdots & \lambda\boldsymbol{x} \\ -\lambda\boldsymbol{x} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & -\lambda\boldsymbol{x} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -\lambda\boldsymbol{x} & \cdots & \mathbf{0} \\ \vdots & \ddots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & -\lambda\boldsymbol{x} \end{pmatrix}.$$

This shows that we can get $k-1$ independent eigenvectors (that is, the columns of Y) corresponding to the eigenvalue λ, hence the result follows. ∎

Corollary 3.4.3. *Let T' be a tree obtained from a tree T by increasing the number of leaves (pendant vertices) attached to the vertex $u \in V(T)$ by $k \geq 2$. Then -2 is an eigenvalue of T' with multiplicity at least $k-1$.*

Proof. Let $T' = T_u \circ H_v^k$, where H is a tree of order 1 and T is a tree of order $n \geq 1$. By Theorem 3.4.2 we know the spectrum of $D(T')$ contains the spectrum of $\mathbb{D}_v(H)$ with multiplicity at least $k-1$. So we consider the characteristic polynomial of $\mathbb{D}_v(H)$ and obtain

$$\Psi_{\mathbb{D}_v(H)} = (x+2).$$

This gives us the result. ∎

As for the adjacency spectrum and the Laplacian spectrum, we study the multiplicities of the "forced" eigenvalues (here, the eigenvalues of $\mathbb{D}_v(H)$) in the distance spectrum when several copies of a tree H are attached to different vertices of a tree G and obtain the following theorem.

Theorem 3.4.4. *Suppose T is a tree obtained from G by joining $k_i \geq 2$ copies of the tree H to the vertices $u_i \in V(G), i = \{1,2,\ldots,l\}$. Then the multiplicity of each of the "forced" eigenvalues in the distance spectrum of T is at least $\sum_{i=1}^{l}(k_i-1)$.*

Proof. Let T be a tree obtained from G by joining the vertex v of each of the $k_i \geq 2$ copies of the tree H to the vertices $u_i \in V(G), i = \{1,2,\ldots,l\}$. Let T, G and H be of order n, m and p respectively. We let the vectors $\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_l$ represent the columns of $D(G)$ corresponding to the vertices $u_1, u_2, \ldots, u_l$ in $V(G)$ respectively. Also, let $\boldsymbol{r}$ denote the column in $D(H)$ corresponding to the vertex $v \in V(H)$.
In order to simplify $D(T)$ we let Q_{k_i} be a $p \times mk_i$ matrix of the form

$$Q_{k_i} = \begin{pmatrix} Q & Q & \cdots & Q \end{pmatrix},$$

where $Q = (\boldsymbol{v}_i + \mathbf{1})\mathbf{1}^T + \mathbf{1}^T\boldsymbol{r}$.
Also, we let D_{k_i} be an $mk_i \times mk_i$ matrix of the form

$$D_{k_i} = \begin{pmatrix} D(H) & R_{u_i}(H) & R_{u_i}(H) & \cdots & R_{u_i}(H) \\ R_{u_i}(H) & D(H) & R_{u_i}(H) & \cdots & R_{u_i}(H) \\ R_{u_i}(H) & R_{u_i}(H) & D(H) & \cdots & R_{u_i}(H) \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ R_{u_i}(H) & R_{u_i}(H) & R_{u_i}(H) & \cdots & D(H) \end{pmatrix}$$

and finally, we let $W_{u_iu_j}, i \neq j$, be an $mk_i \times mk_j$ matrix of the form

$$W_{u_iu_j} = \begin{pmatrix} W & W & \cdots & W \\ \vdots & \vdots & \vdots & \vdots \\ W & W & \cdots & W \end{pmatrix},$$

where $W = R_{u_i}(H) + d(u_i, u_j)J$ and $d(u_i, u_j)$ is the distance from u_i to u_j. Now we can express $D(T)$ as

$$D(T) = \begin{pmatrix} D(G) & Q_{k_1} & Q_{k_2} & \cdots & Q_{k_l} \\ Q_{k_1}^T & D_{k_1} & W_{u_1u_2} & \cdots & W_{u_1u_l} \\ Q_{k_2}^T & W_{u_1u_2} & D_{k_2} & \cdots & W_{u_2u_l} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ Q_{k_l}^T & W_{u_1u_l} & W_{u_2u_l} & \cdots & D_{k_l} \end{pmatrix}.$$

Suppose $\boldsymbol{x}$ is an eigenvector corresponding to an eigenvalue λ of the matrix $\mathbb{D}_v(H)$. We define an $n \times (k_i - 1)$ matrix Y_{k_i} to be of the form

$$Y_{k_i} = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \boldsymbol{x} & \boldsymbol{x} & \boldsymbol{x} & \cdots & \boldsymbol{x} \\ -\boldsymbol{x} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & -\boldsymbol{x} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -\boldsymbol{x} & \cdots & \mathbf{0} \\ \vdots & \ddots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \cdots & -\boldsymbol{x} \end{pmatrix}.$$

So we let Y be the block matrix of the form

$$Y = \begin{pmatrix} O & O & O & \cdots & O \\ Y_{k_1} & O & O & \cdots & O \\ O & Y_{k_2} & O & \cdots & O \\ O & O & Y_{k_3} & \cdots & O \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ O & O & O & \cdots & Y_{k_l} \end{pmatrix}.$$

If we compute $D(T)Y$ we get

$$D(T)Y = \begin{pmatrix} O & O & O & \cdots & O \\ \lambda Y_{k_1} & O & O & \cdots & O \\ O & \lambda Y_{k_2} & O & \cdots & O \\ O & O & \lambda Y_{k_3} & \cdots & O \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ O & O & O & \cdots & \lambda Y_{k_l} \end{pmatrix} = \lambda Y.$$

From the equation $D(T)Y = \lambda Y$, we see that λ is also an eigenvalue of T corresponding to at least $\sum_{i=1}^{l}(k_i - 1)$ linearly independent eigenvectors (that is, the columns of Y). This is true for all eigenvalues of $\mathbb{D}_v(H)$ and hence we obtain our result. ■

Corollary 3.4.5 ([8]). *The multiplicity of the eigenvalue -2 in the distance spectrum of a tree T is at least $l(T) - q(T)$.*

Proof. The proof is analogous to that of Corollary 3.2.5 by considering the fact that K_1 forces the eigenvalue -2. ■

Remark 3.4.6. *Our results shows that we can force the spectrum of $\mathbb{D}_v(T)$ to be in the distance spectrum of an arbitrary tree. Like the Laplacian spectrum, we cannot force every eigenvalue in the distance spectrum. This is because of the well known fact that the distance spectrum of a tree consists of only one positive eigenvalue, while the rest is negative [3, p. 104]. In particular, we cannot force any positive real number. It follows immediately that the spectrum of $\mathbb{D}_v(T)$ consists of only negative eigenvalues. Note that the distance matrix of a tree T of order $n > 1$ is non-singular [21] because*

$$\det(D(T)) = (-1)^{n-1}(2)^{n-2}(n-1).$$

3.5 General remarks

We have proved that when we join two or more copies of a tree to a vertex in another tree, it forces some eigenvalues to be in the spectrum of the resulting tree. However, the converse is not true. For instance, in the case of the adjacency matrix, our results show that the complete graph K_1 of order one is a forcing subtree for the eigenvalue zero. We know that zero is also in the spectrum of a path P_5 of order 5. However, it is clear from the structure of P_5 that the eigenvalue zero was not forced by K_1. Similar examples can be found for the Laplacian and distance spectrum of trees.

3.6 Lower Bounds on the mean multiplicity of eigenvalues

We present a more general case of Corollary 3.2.5. Let T^* be a subtree of a tree T. Suppose $l^*(T^*)$ is the number of copies of T^* in T and $q^*(T^*)$ is the number of vertices in T that are joined to the copies of T^*. For an eigenvalue

λ of $A(T^*)$, it occurs in the spectrum of T with multiplicity at least $l^*(T^*) - q^*(T^*)$. Similar statements can be made for Laplacian and distance spectra of T if we consider the spectra of $L^1(T^* : u)$ and $\mathbb{D}_v(T^*)$ respectively.
We can therefore deduce from the results on "forcing" subtrees and Theorem 3.1.1 that for every real number α that is in the spectrum of some tree, the mean proportion of α in the spectrum of a large random labelled tree is strictly greater than 0. In a more general sense, a lower bound for the mean proportion of an eigenvalue α in the spectrum of a large random tree T is the average number of occurrences of the "forcing" subtree H of α in T. This results is captured in the following corollary.

Corollary 3.6.1. *Let F_α be a "forcing" subtree for an eigenvalue α. Then the mean multiplicity μ_α of α as an eigenvalue of a large random tree T of order n is asymptotically greater than or equal to $C_{F_\alpha} n$, where C_{F_α} is the average proportion of subtrees in T isomorphic to F_α.*

As indicated earlier, the values of C_{F_α} for the above-mentioned families of random trees are known and they are captured in the following theorems.

Theorem 3.6.2 ([38])**.** *Let $\mathbb{T}$ be a family of simply generated trees. Then the mean number of occurrences of a subtree S in a large random simply generated tree T of order n is asymptotically equal to $C_S n$, where*

$$C_S = \frac{1}{\tau} W(S) \rho^{|S|}.$$

Here, ρ and τ are defined as in Section 2.3.

Now let us apply Theorem 3.6.2 to compute lower bounds for the mean proportion of the eigenvalue 0 in the adjacency spectrum of a large random simply generated tree T. This result is shown in Table 3.1.

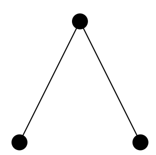


Figure 3.2: The "forcing" subtree F_0 for the eigenvalue 0.

It is important to note that the same results hold for the eigenvalues 1 and -2 in the Laplacian and the distance spectrum, respectively, since they are forced by the same subtree structure, depicted in Figure 3.2.

Simply Generated Trees	$W(F_0)$	τ	ρ	C_{F_0}
Labelled rooted trees	$\frac{1}{2}$	1	$\frac{1}{e}$	$\frac{1}{2e^3} \approx 0.2489$
Plane trees	1	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{32} = 0.03125$
Pruned binary trees	1	1	$\frac{1}{4}$	$\frac{1}{64} = 0.015625$

Table 3.1: Lower bounds for the mean proportion of the eigenvalue 0 in the spectrum of a simply generated tree.

For the case of increasing trees, we shall consider recursive trees and binary increasing trees.

Theorem 3.6.3 ([38]). *The mean number of occurrences of a subtree S in a large random recursive tree T and a large binary increasing tree H of order n is asymptotically equal to $A_S n$ and $B_S n$ respectively, where*

$$A_S = \frac{I(S)}{(|S|+1)!}$$

and

$$B_S = \frac{2I(S)}{(|S|+2)!},$$

where $I(S)$ is the number of increasing labellings of S.

From Theorem 3.6.3, we compute lower bounds for the mean proportion of the eigenvalue 0 in the spectrum of some families of increasing trees and the result is shown in Table 3.2.

Increasing Trees	$I(F_0)$	
Recursive trees	1	$A_{F_0} = \frac{1}{24} \approx 0.04167$
Binary increasing trees	2	$B_{F_0} = \frac{1}{30} \approx 0.03333$

Table 3.2: Lower bounds for the mean proportion of the eigenvalue 0 in the spectrum of an increasing tree.

Remark 3.6.4. *By constructing "forcing" subtrees, we showed that we can force certain real numbers into the spectrum of other trees. Therefore, this idea links the distribution of eigenvalues to that of subtrees in a tree. With this, we deduced lower bounds for the distribution of eigenvalues in some families of random trees. A consequence of this result is the fact that the mean proportion of an eigenvalue in the spectrum of a large random tree is strictly positive. It is therefore an interesting* *problem to find an explicit formula to compute these mean proportions of eigenvalues. Note that the lower bounds are relatively weak since there may exist several non-isomorphic forcing subtrees corresponding to a particular eigenvalue.*

Chapter 4

On the distribution of eigenvalues of simply generated trees

4.1 Introduction

In this chapter, we discuss the distribution of the eigenvalues for the adjacency and Laplacian matrices of simply generated trees. Specifically, we shall focus on computing the mean proportion of an eigenvalue in the spectrum or Laplacian spectrum of these families of trees. Our results in the previous chapter provide evidence of a positive limiting proportion of an eigenvalue in the spectrum of a large simply generated tree. So finding the precise proportion is an interesting problem to consider.

4.2 The distribution of eigenvalues of simply generated trees

We begin by defining a bivariate generating function $F(x,u)$, where x marks the size of the tree and u marks the multiplicity of α as an eigenvalue in the spectrum of the tree. That is,

$$F(x,u) = \sum_{T \in \mathbb{T}} W(T) x^{|T|} u^{N_\alpha(T)}. \tag{4.1}$$

By considering the decomposition of a tree described earlier, we get

$$
\begin{aligned}
F(x,u) &= \sum_{T\in\mathbb{T}} W(T)x^{|T|}\left(u^{N_\alpha(T)} - u^{N_\alpha(T-r)} + u^{N_\alpha(T-r)}\right)\\
&= \sum_{T\in\mathbb{T}} W(T)x^{|T|}u^{N_\alpha(T-r)} + \sum_{T\in\mathbb{T}} W(T)x^{|T|}\left(u^{N_\alpha(T)} - u^{N_\alpha(T-r)}\right)\\
&= \sum_{k\geq 0} w_k \sum_{T_1}\cdots\sum_{T_k}\prod_{j=1}^{k} W(T_j)x^{1+\sum_{j=1}^{k}|T_j|}u^{N_\alpha(T-r)}\\
&\quad + \sum_{T\in\mathbb{T}} W(T)x^{|T|}\left(u^{N_\alpha(T)} - u^{N_\alpha(T-r)}\right).
\end{aligned}
$$

Note that $N_\alpha(T-r) = N_\alpha(T_1) + \cdots + N_\alpha(T_k)$. Therefore

$$
\begin{aligned}
F(x,u) &= \sum_{k\geq 0} xw_k \prod_{j=1}^{k}\left(\sum_{T_j} W(T_j)x^{|T_j|}u^{N_\alpha(T_j)}\right) + \sum_{T\in\mathbb{T}} W(T)x^{|T|}\left(u^{N_\alpha(T)} - u^{N_\alpha(T-r)}\right)\\
&= x\sum_{k\geq 0} w_k F(x,u)^k + \sum_{T\in\mathbb{T}} W(T)x^{|T|}\left(u^{N_\alpha(T)} - u^{N_\alpha(T-r)}\right)\\
&= x\Phi(F(x,u)) + \sum_{T\in\mathbb{T}} W(T)x^{|T|}\left(u^{N_\alpha(T)} - u^{N_\alpha(T-r)}\right). \qquad (4.2)
\end{aligned}
$$

By considering the multiplicity of an eigenvalue α in a tree T as an additive parameter, as defined earlier, the following result is immediate from Theorem 3.6.2.

Corollary 4.2.1. *Let $F(x,1)$ be the ordinary generating function of simply generated trees satisfying the implicit equation $F(x,1) = x\Phi(F(x,1))$. The mean multiplicity $\mu_\alpha(n)$ of an eigenvalue α in the spectrum of a large random simply generated tree of order n is asymptotically equal to nC_α where*

$$
C_\alpha = \left(\frac{1}{\tau}\right)\sum_{T\in\mathbb{T}} W(T)\rho^{|T|}\left(N_\alpha(T) - N_\alpha(T-r)\right) \qquad (4.3)
$$

and $\tau = F(\rho,1)$.

Proof. The mean multiplicity $\mu_\alpha(n)$ of an eigenvalue α in the spectrum of a simply generated tree of order n is given by

$$
\mu_\alpha(n) = \frac{[x^n]F_u(x,1)}{[x^n]F(x,1)},
$$

where

$$
F_u(x,1) = \left.\frac{\partial F(x,u)}{\partial u}\right|_{u=1}
$$

and $[x^n]F_u(x,1)$ is the coefficient of x^n in the generating function $F_u(x,1)$. We therefore compute

$$\begin{aligned} F_u(x,1) &= x\Phi'(F(x,1))F_u(x,1) + \sum_{T\in\mathbb{T}} W(T)x^{|T|}\left(N_\alpha(T) - N_\alpha(T-r)\right) \\ &= \left(\frac{1}{1-x\Phi'(F(x,1))}\right)\sum_{T\in\mathbb{T}} W(T)x^{|T|}\left(N_\alpha(T) - N_\alpha(T-r)\right). \end{aligned} \tag{4.4}$$

Also, we have

$$\begin{aligned} F_x(x,1) &= \Phi(F(x,1)) + x\Phi'(F(x,1))F_x(x,1) \\ &= \frac{\Phi(F(x,1))}{1-x\Phi'(F(x,1))}. \end{aligned} \tag{4.5}$$

So by equations (4.4) and (4.5) we get

$$\begin{aligned} F_u(x,1) &= \left(\frac{xF_x(x,1)}{x\Phi(F(x,1))}\right)\sum_{T\in\mathbb{T}} W(T)x^{|T|}\left(N_\alpha(T) - N_\alpha(T-r)\right) \\ &= \left(\frac{xF_x(x,1)}{F(x,1)}\right)\sum_{T\in\mathbb{T}} W(T)x^{|T|}\left(N_\alpha(T) - N_\alpha(T-r)\right). \end{aligned}$$

As $x \to \rho^-$, we have

$$\begin{aligned} F_u(x,1) &\sim xF_x(x,1)\left(\frac{1}{F(\rho,1)}\right)\sum_{T\in\mathbb{T}} W(T)\rho^{|T|}\left(N_\alpha(T) - N_\alpha(T-r)\right) \\ &\sim xF_x(x,1)\left(\frac{1}{\tau}\right)\sum_{T\in\mathbb{T}} W(T)\rho^{|T|}\left(N_\alpha(T) - N_\alpha(T-r)\right) \\ &\sim xF_x(x,1)\cdot C_\alpha \end{aligned}$$

where

$$C_\alpha = \left(\frac{1}{\tau}\right)\sum_{T\in\mathbb{T}} W(T)\rho^{|T|}\left(N_\alpha(T) - N_\alpha(T-r)\right). \tag{4.6}$$

Therefore the mean multiplicity μ_α of an eigenvalue α in the spectrum of a simply generated tree of order n is given by

$$\begin{aligned} \mu_\alpha = \frac{[x^n]\,F_u(x,1)}{[x^n]\,F(x,1)} &\sim \frac{[x^n]\,xF_x(x,1)\cdot C_\alpha}{[x^n]\,F(x,1)} \\ &= \frac{n\,[x^n]\,F(x,1)}{[x^n]\,F(x,1)}C_\alpha \\ &= nC_\alpha. \end{aligned} \tag{4.7}$$

■

Remark 4.2.2. *It is not obvious that the sum*

$$\sum_{T \in \mathbb{T}} W(T)\rho^{|T|} \left(N_\alpha(T) - N_\alpha(T-r)\right)$$

converges. However, since $N_\alpha(T) - N_\alpha(T-r) \in \{-1, 0, 1\}$ *as observed in Section 2.6 it follows that the sum converges absolutely.*

Remark 4.2.3. *The formula for* C_α *can also be derived from general results on additive functionals, see for example Theorem 1.3 in [27].*

Next we show that one can determine the value of C_α for a given eigenvalue α by solving a system of functional equations.

Theorem 4.2.4. *Let* T *denote a simply generated tree with root* r*. Suppose* $\Psi(T,z)$ *and* $\Psi_r(T,z)$ *are the characteristic polynomials of* T *and* $T-r$ *respectively and define a generating function* $H_t(x)$ *for every* $t \in \mathbb{R} \cup \{\infty\}$ *by*

$$H_t(x) = \sum_{\frac{\Psi_r(T,\alpha)}{\Psi(T,\alpha)} = t} W(T)x^{|T|}.$$

Then the mean proportion C_α *of an eigenvalue* α *in the spectrum of a large simply generated tree is given by*

$$C_\alpha = \frac{1}{\tau}\left(H_\infty(\rho) - H_0(\rho)\right)$$

where the values for $H_\infty(\rho)$ *and* $H_0(\rho)$ *are obtained by solving the following system of functional equations:*

$$H_0(\rho) = \tau - \rho\Phi(\tau - H_\infty(\rho)),$$

$$\sum_{t \neq 0} H_t(\rho) y^{\alpha - \frac{1}{t}} = \rho\Phi\left(\sum_{u \geq 0} H_u(\rho) y^u\right).$$

Remark 4.2.5. *In the second equation,* y *mainly acts as a formal variable. Thus we actually have an infinite system of equations for the values* $H_t(\rho)$*.*

Proof of Theorem 4.2.4. Let α be a fixed eigenvalue of trees. If we define a generating function $H_t(x)$ to be given by

$$H_t(x) = \sum_{\frac{\Psi_r(T,\alpha)}{\Psi(T,\alpha)} = t} W(T)x^{|T|} \tag{4.8}$$

then by the Cauchy Interlacing Theorem and our results on the types of trees based on the value of the ratio $\frac{\Psi_r(T,\alpha)}{\Psi(T,\alpha)}$ (see Section 2.6) we get

$$\begin{aligned} C_\alpha &= \frac{1}{\tau}\left(\sum_{\frac{\Psi_r(T,\alpha)}{\Psi(T,\alpha)}=\infty} W(T)\rho^{|T|} - \sum_{\frac{\Psi_r(T,\alpha)}{\Psi(T,\alpha)}=0} W(T)\rho^{|T|}\right) \\ &= \frac{1}{\tau}\left(H_\infty(\rho) - H_0(\rho)\right) \end{aligned} \tag{4.9}$$

and

$$F(x) = \sum_t H_t(x). \tag{4.10}$$

From the characterisation of a type zero tree in Theorem 2.6.3 we get the following functional equation:

$$H_0(x) = x\Phi(F(x)) - x\Phi(F(x) - H_\infty(x)).$$

Note that $x\Phi(F(x))$ denote a root and a sequence of rooted trees and $x\Phi(F(x) - H_\infty(x))$ denote a root and a sequence of rooted trees which are not type pole. So the difference gives us type zero trees.
Now, we have

$$H_0(\rho) = \tau - \rho\Phi(\tau - H_\infty(\rho)).$$

Also, from Theorem 2.6.2 we obtain that for a given α and a tree T with branches $T_1, T_2, \ldots, T_d$

$$\frac{\Psi_r(T,\alpha)}{\Psi(T,\alpha)} = \frac{1}{\alpha - S(\alpha)}$$

where

$$S(\alpha) = \sum_{j=1}^{d} \frac{\Psi_{v_j}(T_j,\alpha)}{\Psi(T_j,\alpha)}.$$

Thus

$$\frac{\Psi_r(T,\alpha)}{\Psi(T,\alpha)} = t$$

if and only if $S(\alpha) = \alpha - \frac{1}{t}$. This yields the following functional equation

$$H_t(x) = \left[y^{\alpha-\frac{1}{t}}\right] x\Phi\left(\sum_{u\geq 0} H_u(x)y^u\right), \quad t \neq 0.$$

Therefore, to compute C_α for a given α we set $x = \rho$ in the following system of functional equations:

$$H_0(x) = x\Phi(F(x)) - x\Phi(F(x) - H_\infty(x)), \tag{4.11}$$

$$\sum_{t\neq 0} H_t(x) y^{\alpha - \frac{1}{t}} = x\Phi\left(\sum_{u\geq 0} H_u(x) y^u\right), \tag{4.12}$$

and solve for $H_0(\rho)$ and $H_\infty(\rho)$. Thus we have the following system:

$$H_0(\rho) = \tau - \rho\Phi(\tau - H_\infty(\rho)), \tag{4.13}$$

$$\sum_{t\neq 0} H_t(\rho) y^{\alpha - \frac{1}{t}} = \rho\Phi\left(\sum_{u\geq 0} H_u(\rho) y^u\right). \tag{4.14}$$

∎

Remark 4.2.6. *Solving this system of infinitely many equations may, in principle, be very difficult. However, resorting to computational methods will be an essential tool to obtain the required results. Also, we shall see later that for the special eigenvalue $\alpha = 0$, this system reduces to solving two equations.*

Let us consider a sketch of the algorithm used to solve the system of functional equations.

Algorithm 4.2.7. *There are three main procedures for this algorithm, namely*

1. *Consider the RHS of equation* (4.14)*;*

   I. *Initialise by setting* $L = [(u, H_u(\rho)) : H_u(\rho) = 0 \quad \forall\, u]$

   II. *If Φ is an infinite series then fix an upper limit M for the sum and simplify to obtain a polynomial instead of Φ*

   III. *Extract the powers of y and its coefficients in*

   $$P(y) = \rho\Phi\left(\sum_{u\geq 0} H_u(\rho) y^u\right)$$

   to form a new list

   $$L_1 = [(u, K_u(\rho)) : K_u(\rho) = \textit{coefficient of } y^u]$$

2. *Consider equation* (4.13) *and the LHS of equation* (4.14)*;*

I. *Let L_2 be an empty list, i.e. $L_2 = []$*

II. *For each element $(u, K_u(\rho))$*

A. *If $u \neq \alpha$ then*

a. *Compute $t = \frac{1}{\alpha - u}$*

b. *Set $H_t(\rho) = K_u(\rho)$*

c. *Append $(t, H_t(\rho))$ to L_2*

B. *else:*

a. *Set $t = \infty$ and $H_\infty(\rho) = K_\alpha(\rho)$*

b. *Solve for $H_0(\rho)$ from equation* (4.13)

c. *Append $(0, H_0(\rho))$ and $(\infty, H_\infty(\rho))$ to L_2*

III. *Print from L_2 the values $H_0(\rho), H_\infty(\rho))$ and $\sum_t H_t(\rho)$*

3. *Repeat the process by setting $L = L_2$*

Remark 4.2.8. *It is important to note that for all t the value of $H_t(\rho)$ increases after every iteration of this algorithm. Further, we know that the sum $\sum_t H_t(\rho)$ is bounded above by τ. This implies that the series converges. However, it converges very slowly and will require a long period of time to obtain the desired results. In order to tackle this problem, one can fix the value of $H_\infty(\rho)$ and for all $t \neq \infty$ update their corresponding values $H_t(\rho)$ for each iteration. That is, at procedure* 2*IIBa of Algorithm 4.2.7 we set $H_\infty(\rho)$ to be equal to a constant K. By doing this and checking the value of the sum $\sum_t H_t(\rho)$, one can obtain lower and upper bounds for $H_\infty(\rho)$ which in turn gives us $H_0(\rho)$.*

Next we present the system of infinite functional equations for each of the above-mentioned classes of simply generated trees and also state the results of the application of Algorithm 4.2.7 to solve these systems to obtain the limit proportion for specific eigenvalues.

4.2.1 Plane trees

Suppose we let $\mathbb{T}_p$ denote the set of all plane trees and consider a bivariate generating function $\mathcal{P}(x, u)$, where u marks $N_\alpha(T)$, to be given by

$$\mathcal{P}(x, u) = \sum_{T \in \mathbb{T}_p} x^{|T|} u^{N_\alpha(T)}.$$

Then we obtain that the mean multiplicity μ_α of an eigenvalue α in the spectrum of a randomly generated plane tree T of order n is asymptotically given by nC_α, where by equation (4.6) we get

$$\begin{aligned} C_\alpha &= \left(\frac{1}{\tau}\right) \sum_{T\in\mathbb{T}_p} W(T)\rho^{|T|} \left(N_\alpha(T) - N_\alpha(T-r)\right) \\ &= 2\sum_{T\in\mathbb{T}_p} \left(\frac{1}{4}\right)^{|T|} \left(N_\alpha(T) - N_\alpha(T-r)\right). \end{aligned} \tag{4.15}$$

If we define a generating function $H_t(x)$ as in the previous section, to be given by

$$H_t(x) = \sum_{\frac{\Psi_r(T,\alpha)}{\Psi(T,\alpha)}=t} x^{|T|}, \tag{4.16}$$

then we get that

$$\begin{aligned} C_\alpha &= \frac{1}{\tau}\left(H_\infty(\rho) - H_0(\rho)\right) \\ &= 2\left(H_\infty\left(\frac{1}{4}\right) - H_0\left(\frac{1}{4}\right)\right). \end{aligned} \tag{4.17}$$

Also, by Theorem 2.6.2 and the characterisation of a type zero simply generated tree in Theorem 2.6.3 we obtain the following system of functional equations

$$H_0(x) = \frac{x}{1-\mathcal{P}(x)} - \frac{x}{1-\mathcal{P}(x)+H_\infty(x)}$$

and

$$\begin{aligned} \sum_{t\neq 0} H_t(x) y^{\alpha-\frac{1}{t}} &= \frac{x}{1-\sum_{u\geq 0} H_u(x)y^u} \\ &= x\sum_{k\geq 0}\left(\sum_{u\geq 0} H_u(x)y^u\right)^k. \end{aligned}$$

If we set $x=\rho=\frac{1}{4}$ in the system of functional equations we obtain

$$\begin{aligned} H_0\left(\frac{1}{4}\right) &= \frac{1}{2} - \frac{\frac{1}{4}}{1-\left(\frac{1}{2}-H_\infty(\frac{1}{4})\right)} \\ &= \frac{1}{2} - \frac{1}{2+4H_\infty(\frac{1}{4})} \end{aligned} \tag{4.18}$$

and

$$\sum_{t\neq 0} H_t\left(\frac{1}{4}\right)y^{\alpha-\frac{1}{t}} = \frac{1}{4}\sum_{k\geq 0}\left(\sum_{u\geq 0} H_u\left(\frac{1}{4}\right)y^u\right)^k . \tag{4.19}$$

We resorted to computational methods to solve this system to obtain the mean proportion of some eigenvalues. The result is shown in Table 4.1 for two examples. A lower bound is given in the first row, an upper bound in the second row.

α	$H_\infty(\frac{1}{4})$	$H_0(\frac{1}{4})$	$\sum_t H_t(\frac{1}{4})$	C_α
1	0.0864002589	0.0736700382	0.4999461440	0.0254604415
	0.0864258900	0.0736886719	0.5000090998	0.0254744362
$\sqrt{2}$	0.0546600050	0.0492734328	0.4999982592	0.0107731443
	0.0546900050	0.0492978100	0.5000262824	0.0107843899

Table 4.1: The mean proportion of eigenvalues α in a large randomly generated plane tree

From Table 4.1 we can deduce that C_1 and $C_{\sqrt{2}}$ are within the intervals

$$(0.0254604415, 0.0254744362) \quad \text{and} \quad (0.0107731443, 0.0107843899)$$

respectively. Hence, we obtain that approximately 1.1% and 2.5% of the spectrum of a large random plane tree consist of the eigenvalues $\sqrt{2}$ and 1 respectively.

4.2.2 Labelled rooted trees

We include the multiplicity of an eigenvalue α in the spectrum a tree T, denoted by $N_\alpha(T)$, into the generating function for labelled rooted trees. So we define a bivariate generating function $L(x,u)$, where u marks $N_\alpha(T)$, by

$$L(x,u) = \sum_{T\in\mathbb{T}_l} \frac{x^{|T|}u^{N_\alpha(T)}}{|T|!}.$$

From equation (4.7) we can deduce that the mean multiplicity μ_α of an eigenvalue α in the spectrum of a large random labelled rooted tree T of order n is asymptotically nC_α, where

$$C_\alpha = \sum_{T\in\mathbb{T}_l} \frac{e^{-|T|}}{|T|!}\left(N_\alpha(T) - N_\alpha(T-r)\right).$$

Setting

$$H_t(x) = \sum_{\frac{\Psi_r(T,\alpha)}{\Psi(T,\alpha)}=t} \frac{x^{|T|}}{|T|!},$$

we get

$$C_\alpha = H_\infty\left(\frac{1}{e}\right) - H_0\left(\frac{1}{e}\right). \tag{4.20}$$

It follows from Theorem 2.6.3 and Theorem 4.3.1 that we can determine C_α by solving the following system of functional equations:

$$\begin{aligned} H_0\left(\frac{1}{e}\right) &= \frac{1}{e}\left(e^{L(\frac{1}{e})} - e^{L(\frac{1}{e})-H_\infty(\frac{1}{e})}\right) \\ &= \frac{1}{e}\left(e - e^{1-H_\infty(\frac{1}{e})}\right) \\ &= 1 - e^{-H_\infty(\frac{1}{e})} \end{aligned} \tag{4.21}$$

and

$$\begin{aligned} \sum_{t\neq 0} H_t\left(\frac{1}{e}\right) y^{\alpha-\frac{1}{t}} &= \frac{1}{e}\exp\left(\sum_{u\geq 0} H_u\left(\frac{1}{e}\right) y^u\right) \\ &= \frac{1}{e}\prod_u\left(\sum_{k\geq 0}\frac{1}{k!} H_u\left(\frac{1}{e}\right)^k y^{uk}\right). \end{aligned} \tag{4.22}$$

By solving this system numerically using Algorithm 4.2.7 we obtain the following results shown in Table 4.2. Again, upper and lower bounds are provided.

α	$H_\infty(\frac{1}{e})$	$H_0(\frac{1}{e})$	$\sum_t H_t(\frac{1}{e})$	C_α
1	0.2137539489	0.1924529416	0.9995348193	0.0213010073
	0.2137549489	0.1924537491	1.0005387585	0.0213011998

Table 4.2: The mean proportion of eigenvalue 1 in a large random labelled rooted tree

We can deduce from Table 4.2 that C_1 is within the interval

$$(0.0213010073, 0.0213011998),$$

and this implies that approximately 2.1% of the spectrum of a large labelled rooted tree consist of the eigenvalue 1.

4.2.3 Pruned d-ary trees

Similar to plane trees and labelled rooted trees, we define a bivariate generating function $\mathfrak{D}(x,u)$, where u marks $N_\alpha(T)$, as

$$\mathfrak{D}(x,u) = \sum_{T\in\mathbb{T}_d} x^{|T|} u^{N_\alpha(T)}.$$

It follows from equation (4.7) that the average multiplicity μ_α of an eigenvalue α in the spectrum of a large randomly generated pruned d-ary tree is asymptotically nC_α, where

$$\begin{aligned} C_\alpha &= \left(\frac{1}{\tau}\right) \sum_{T\in\mathbb{T}_d} \rho^{|T|} \left(N_\alpha(T) - N_\alpha(T-r)\right) \\ &= (d-1) \sum_{T\in\mathbb{T}_d} \left(\frac{(d-1)^{d-1}}{d^d}\right)^{|T|} \left(N_\alpha(T) - N_\alpha(T-r)\right). \end{aligned}$$

In order to compute C_α, we set

$$H_t(x) = \sum_{\frac{\Psi_r(T,\alpha)}{\Psi(T,\alpha)}=t} x^{|T|}$$

and get

$$C_\alpha = (d-1)\left(H_\infty(\rho) - H_0(\rho)\right),$$

where $\rho = \frac{(d-1)^{d-1}}{d^d}$.

We substitute τ and ρ into the functional equations (4.13) and (4.14) and obtain the following:

$$H_0(\rho) = \frac{1}{d-1} - \frac{(d-1)^{d-1}}{d^d}\left[\frac{d}{d-1} - H_\infty(\rho)\right]^d, \tag{4.23}$$

$$\sum_{t\neq 0} H_t(\rho) y^{\alpha-\frac{1}{t}} = \frac{(d-1)^{d-1}}{d^d}\left[1 + \sum_u H_u(\rho) y^u\right]^d. \tag{4.24}$$

By using Algorithm 4.2.7, one can solve this infinite system numerically. Next we present the results from computing C_α for $\alpha = 1$ and $d = 2, 3$.

4.2.3.1 Pruned binary trees

In this section, we determine the value of the average proportion C_1 of the eigenvalue 1 in the spectrum of a large random pruned binary tree. From our calculations in the general d-ary case we obtain $\tau = 1$ and $\rho = \frac{1}{4}$ for $d = 2$.

So if we set $d = 2$ in equations (4.23) and (4.24) and solve them using Algorithm 4.2.7 to obtain the following results shown in Table 4.3. Again, upper and lower bounds are provided in the first and second rows respectively.

α	$H_\infty(\frac{1}{4})$	$H_0(\frac{1}{4})$	$\sum_t H_t(\frac{1}{4})$	C_α
1	0.23729000	0.22321336	0.99990096	0.01407663
	0.23755000	0.22344250	1.00061319	0.01410750

Table 4.3: The mean proportion of the eigenvalue 1 in a large random pruned binary tree

It can be observed from Table 4.3 that C_1 is within the interval

$$(0.01407663, 0.01410750).$$

Therefore, we can conclude that on average approximately 1.4% of the spectrum of a large random pruned binary tree is the eigenvalue 1.

4.2.3.2 Pruned ternary trees

This section is devoted to determining the value of C_1 for pruned ternary trees. For $d = 3$, we get

$$\tau = \frac{1}{2} \quad \text{and} \quad \rho = \frac{2^2}{3^3} = \frac{4}{27}.$$

Similar to pruned binary trees, we set $d = 3$ in equations (4.23) and (4.24) and solve them numerically using Algorithm 4.2.7 to obtain the following results in Table 4.4.

α	$H_\infty(\frac{4}{27})$	$H_0(\frac{4}{27})$	$\sum_t H_t(\frac{4}{27})$	C_α
1	0.11979950	0.10323278	0.49998289	0.03313345
	0.11989903	0.10322673	0.50007337	0.03333366

Table 4.4: The mean proportion of the eigenvalue 1 in a large random ternary tree

It can be deduced from Table 4.4 that approximately 3.3% of the spectrum a large random ternary tree consist of the eigenvalue 1.

4.3 The proportion of the eigenvalue 0 in the spectrum of a simply generated tree

In this section, we focus on the mean proportion of the eigenvalue 0, thus computing C_0, in the spectrum of a large random simply generated tree. It is a well known fact that a tree T is bipartite and its spectrum is symmetric about the origin. In particular, if λ is an eigenvalue with multiplicity m then $-\lambda$ is also an eigenvalue with multiplicity m. It then follows that if a tree T has an odd or even number of vertices then the multiplicity of the eigenvalue 0 is also odd or even respectively. With this fact, we know that if $N_0(T)$ is odd then $N_0(T-r)$ is even and vice versa. This implies that $N_0(T) \neq N_0(T-r)$ for a tree T. Hence by the Cauchy Interlacing Theorem (Theorem 2.2.4), we obtain that the term $N_\alpha(T) - N_\alpha(T-r)$ is either -1 or 1. Therefore, for the eigenvalue 0 a simply generated tree can be either a type zero or a type pole tree. Thus,

$$F(x) = H_0(x) + H_\infty(x).$$

In view of this observation we obtain the following characterisation for a type pole tree.

Theorem 4.3.1. *A tree T is a type pole if and only if all of its branches are type zero.*

Proof. The proof of this theorem follows directly from Theorem 2.6.3 and considering the fact that there is no type $\mathcal{C}$ tree with respect to the eigenvalue 0. ∎

As a consequence of Theorem 4.3.1, we have the following functional equation

$$H_\infty(x) = x\Phi(F(x) - H_\infty(x)). \tag{4.25}$$

Now, to compute C_0 we set $x = \rho$ in the functional equations (4.12) and (4.25) and solve them simultaneously. Thus,

$$H_0(\rho) = \tau - \rho\Phi(\tau - H_\infty(\rho)), \tag{4.26}$$

$$H_\infty(\rho) = \rho\Phi(\tau - H_\infty(\rho)), \tag{4.27}$$

and these yield

$$\begin{aligned} C_0 &= \frac{1}{\tau}\left(H_\infty(\rho) - H_0(\rho)\right) \\ &= \frac{1}{\tau}\left(2H_\infty(\rho) - \tau\right). \end{aligned} \tag{4.28}$$

Let us now proceed to determining the value of C_0 for the above mentioned classes of simply generated trees.

4.3.1 Plane trees

Let us consider a large random plane tree and determine the average proportion of the eigenvalue 0 in its spectrum. Recall that for plane trees we have $\tau = \frac{1}{2}, \rho = \frac{1}{4}$ and $\Phi(t) = \frac{1}{1-t}$. So from equations (4.26) and (4.27) we obtain

$$H_0\left(\frac{1}{4}\right) = \frac{1}{2} - \frac{1}{2 + 4H_\infty(\frac{1}{4})}, \tag{4.29}$$

$$H_\infty\left(\frac{1}{4}\right) = \frac{1}{2 + 4H_\infty(\frac{1}{4})}. \tag{4.30}$$

From equation (4.30) we get

$$\begin{aligned} 4H_\infty(\frac{1}{4})^2 + 2H_\infty(\frac{1}{4}) - 1 = 0& \\ H_\infty(\frac{1}{4}) &= \frac{-2 \pm \sqrt{20}}{8} \\ &= \frac{-1 \pm \sqrt{5}}{4}. \end{aligned}$$

We have that $H_\infty(\frac{1}{4}) = \frac{\sqrt{5}-1}{4}$. So

$$\begin{aligned} H_0(\frac{1}{4}) &= \frac{1}{2} - \frac{\sqrt{5}-1}{4} \\ &= \frac{3-\sqrt{5}}{4} \end{aligned}$$

and hence

$$\begin{aligned} C_0 &= 2\left(\frac{\sqrt{5}-1}{4} - \frac{3-\sqrt{5}}{4}\right) \\ &= \sqrt{5}-2 \\ &= 0.2360679774998. \end{aligned}$$

This means that for a large randomly generated plane tree T approximately 23.6%, on average, of its spectrum consist of the eigenvalue 0.

4.3.2 Labelled rooted trees

This section presents the result on the mean proportion of the eigenvalue 0 in the spectrum of a large random labelled rooted tree. We know from the generating function $L(x)$ of labelled rooted trees that $\tau = 1, \rho = \frac{1}{e}$ and $\Phi(t) = e^t$. So substituting them into equations (4.26) and (4.27) yields

$$H_0\left(\frac{1}{e}\right) = 1 - e^{-H_\infty(\frac{1}{e})}, \tag{4.31}$$

$$H_\infty\left(\frac{1}{e}\right) = e^{-H_\infty(\frac{1}{e})}. \tag{4.32}$$

Definition 4.3.2. *The Lambert-W function is defined by the equation*

$$W(x)e^{W(x)} = x,$$

for any complex number x.

By the definition of the Lambert-W function we have that

$$W(1) = e^{-W(1)}.$$

Comparing to equation (4.32) gives us $H_\infty(\frac{1}{e}) = W(1) \approx 0.567143$. Therefore we get

$$\begin{aligned} C_0 &= 2H_\infty\left(\frac{1}{e}\right) - 1 \\ &= 2W(1) - 1 \\ &\approx 0.134287. \end{aligned}$$

This implies that on average approximately 13.4% of the spectrum of labelled rooted trees is the eigenvalue 0.

4.3.3 Pruned d-ary trees

In this section, we compute the value of C_0 for a large pruned d-ary tree. We know that we can obtain this value by setting $\tau = \frac{1}{d-1}, \rho = \frac{(d-1)^{d-1}}{d^d}$ and $\Phi(t) = (1+t)^d$ in equations (4.26) and (4.27) and solving them simultaneously. Thus we solve

$$H_0(\rho) = \frac{1}{d-1} - \frac{(d-1)^{d-1}}{d^d}\left[\frac{d}{d-1} - H_\infty(\rho)\right]^d, \tag{4.33}$$

$$H_\infty(\rho) = \frac{(d-1)^{d-1}}{d^d}\left[\frac{d}{d-1} - H_\infty(\rho)\right]^d \tag{4.34}$$

simultaneously to get the value for $H_\infty(\rho)$ and substitute it into the equation

$$C_0 = (d-1)\left(2H_\infty(\rho) - \frac{1}{d-1}\right)$$

for a given d.

Now, let us consider specific cases of pruned d-ary trees.

4.3.3.1 Pruned binary trees

In this section, we determine the value of C_0 for pruned binary trees. Recall that $\tau = 1, \rho = \frac{1}{4}$ and $\Phi(t) = (1+t)^2$.

So by equations (4.33) and (4.34) we obtain the functional equations

$$H_0\left(\frac{1}{4}\right) = 1 - \frac{1}{4}\left(2 - H_\infty\left(\frac{1}{4}\right)\right)^2, \tag{4.35}$$

$$H_\infty\left(\frac{1}{4}\right) = \frac{1}{4}\left(2 - H_\infty\left(\frac{1}{4}\right)\right)^2. \tag{4.36}$$

From equation (4.36) we get

$$\begin{aligned}
4H_\infty\left(\frac{1}{4}\right) &= 4 - 4H_\infty\left(\frac{1}{4}\right) + H_\infty\left(\frac{1}{4}\right)^2 \\
H_\infty\left(\frac{1}{4}\right)^2 - 8H_\infty\left(\frac{1}{4}\right) + 4 &= 0 \\
H_\infty\left(\frac{1}{4}\right) &= 4 \pm 2\sqrt{3}.
\end{aligned}$$

Therefore, we have

$$\begin{aligned}
C_0 &= 2(4 - 2\sqrt{3}) - 1 \\
&= 7 - 4\sqrt{3} \\
&= 0.07179677.
\end{aligned}$$

This implies that on average approximately 7.2% of the spectrum of a large random pruned binary tree is the eigenvalue 0.

4.3.3.2 Pruned ternary trees

In this section, we focus on pruned ternary trees and determine the value of C_0. We know that $\tau = \frac{1}{2}$ and $\rho = \frac{4}{27}$.
Similar to pruned binary trees, we set $d = 3$ in equations (4.33) and (4.34) and these yield

$$H_0\left(\frac{4}{27}\right) = \frac{1}{2} - \frac{4}{27}\left(\frac{3}{2} - H_\infty\left(\frac{4}{27}\right)\right)^3, \tag{4.37}$$

$$H_\infty\left(\frac{4}{27}\right) = \frac{4}{27}\left(\frac{3}{2} - H_\infty\left(\frac{4}{27}\right)\right)^3. \tag{4.38}$$

From equation (4.38) we get

$$\begin{aligned}
27H_\infty\left(\frac{4}{27}\right) &= 4\left(\frac{27}{8} - \frac{27}{4}H_\infty\left(\frac{4}{27}\right) + \frac{9}{2}H_\infty\left(\frac{4}{27}\right)^2 - H_\infty\left(\frac{4}{27}\right)^3\right) \\
0 &= \frac{27}{2} - 54H_\infty\left(\frac{4}{27}\right) + 18H_\infty\left(\frac{4}{27}\right)^2 - 4H_\infty\left(\frac{4}{27}\right)^3 \\
0 &= 27 - 108H_\infty\left(\frac{4}{27}\right) + 36H_\infty\left(\frac{4}{27}\right)^2 - 8H_\infty\left(\frac{4}{27}\right)^3 \\
H_\infty\left(\frac{4}{27}\right) &= \frac{3}{2}\left(\sqrt[3]{\frac{\sqrt{13}-3}{2}} - \frac{1}{\sqrt[3]{\frac{\sqrt{13}-3}{2}}} + 1\right) \\
&= 0.2734024892.
\end{aligned}$$

Note that the other two solutions of equation (4.38) are complex numbers. Therefore we have

$$\begin{aligned}
C_0 &= 2\left(2(0.2734024892) - \frac{1}{2}\right) \\
&= 0.0936099567
\end{aligned}$$

and this implies that about 9.4% of the spectrum of a large pruned ternary tree consist of the eigenvalue 0.

4.4 The distribution of Laplacian eigenvalues of simply generated trees

In this section, we deal with the distribution of eigenvalues in the Laplacian spectrum of simply generated trees analogous to results in Section 4.2. Here we shall consider planted simply generated trees, which are simply generated trees with a hidden vertex attached to its root by an edge. Thus for a simply generated tree T with root r, we consider the spectrum of $L^1(T:r)$. In order to study the distribution of the eigenvalues in the Laplacian spectrum, we employ the same approach as for the adjacency spectrum and consider planted simply generated trees. As mentioned earlier (see Remark 2.6.4), for large n, considering planted simply generated trees has little influence on the multiplicity of eigenvalues.

So we let $G(x,u)$ be a bivariate generating function where x marks the size of the planted simply generated tree (excluding the hidden vertex) and u marks the multiplicity of α as an eigenvalue in the Laplacian spectrum. Thus

$$G(x,u) = \sum_{T\in\mathbb{T}^*} W(T)x^{|T|}u^{N_\alpha(T)},$$

where $\mathbb{T}^*$ is the set of all planted trees from a simply generated family. Note that $G(x) = G(x,1)$. By the same calculation as in Section 4.2 we get that the mean multiplicity of an eigenvalue α in the Laplacian spectrum of a planted simply generated tree of order n is asymptotically given by nC_α, where

$$C_\alpha = \left(\frac{1}{\tau}\right) \sum_{T\in\mathbb{T}^*} W(T)\rho^{|T|}\Big(N_\alpha(T) - N_\alpha(T-r)\Big).$$

Note that the constants τ and ρ are obtained in the same way as described in Section 4.2.

Next, we focus on computing the value of C_α for a given α. By applying the Cauchy Interlacing Theorem, we get that $N_\alpha(T) - N_\alpha(T-r)$ evaluates to $-1, 0$ or 1. We recall some notations. We let $\Psi(T,z)$ and $\Psi_r(T,z)$ be the characteristic polynomials (with respect to the Laplacian matrix) of the trees T and $T-r$ respectively. Based on the value of $N_\alpha(T) - N_\alpha(T-r)$ and the value of the ratio $\frac{\Psi_r(T,z)}{\Psi(T,z)}$ evaluated at $z=\alpha$ we get three types of planted simply generated trees. Namely, type zero, type pole and type C as defined in Section 4.2.

Let $L^1(T : r)$ be the Laplacian matrix of a planted tree T of order n with m distinct eigenvalues, i.e. $\beta_1, \ldots, \beta_m$. For an eigenvalue β_i, we let its eigenspace be $\xi(\beta_i)$ and let $\boldsymbol{y}_j, 1 \leq j \leq k$, be its corresponding orthonormal eigenvectors. If we set $Q_i, 1 \leq i \leq m$, to be the matrix

$$Q_i = \boldsymbol{y}_1\boldsymbol{y}_1^T + \boldsymbol{y}_2\boldsymbol{y}_2^T + \cdots + \boldsymbol{y}_k\boldsymbol{y}_k^T,$$

and let $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_n\}$ be the natural basis vectors of $\mathbb{R}^n$, then we call the numbers $\gamma_{ij} = ||Q_i e_j||, 1 \leq i \leq m$ and $1 \leq j \leq n$, the Laplacian angles of the tree T. The following theorem presents the relationship between the angles of T and $\frac{\Psi_r(T,z)}{\Psi(T,z)}$.

Theorem 4.4.1. *Let T be a planted tree with root r. Suppose $\beta_1, \beta_2, \ldots \beta_m$, are the distinct eigenvalues of T and γ_{ij} are its angles. Then*

$$\frac{\Psi_r(T,z)}{\Psi(T,z)} = \sum_{i=1}^{m} \frac{\gamma_{ir}^2}{z - \beta_i},$$

where $\gamma_{ir} = ||Q_i \boldsymbol{e}_r||$ and $\boldsymbol{e}_r$ is the natural basis vector of $\mathbb{R}^n$ with respect to the root r.

Proof. Let $L^1(T : r)$ be the Laplacian matrix of a planted tree T. We use the well known fact that for a matrix M, it adjugate $\text{adj}(M)$ is equal to its determinant $\det(M)$ times its inverse M^{-1}. So we get

$$\text{adj}(Iz - L^1(T : r)) = \det(Iz - L^1(T : r))(Iz - L^1(T : r))^{-1}.$$

Note that

$$L^1(T : r) = \sum_{i=1}^{m} \beta_i Q_i.$$

So we get

$$\begin{aligned}
\text{adj}(Iz - L^1(T : r)) &= \Psi_{L^1(T:r)}(z) \sum_{i=1}^{m} \frac{1}{z - \beta_i} Q_i \\
\boldsymbol{e}_r^T \text{adj}(Iz - L^1(T : r))\boldsymbol{e}_r &= \Psi_{L^1(T:r)}(z) \sum_{i=1}^{m} \frac{1}{z - \beta_i} \boldsymbol{e}_r^T Q_i \boldsymbol{e}_r \\
\Psi_{L^1(T-r:N(r))} &= \Psi_{L^1(T:r)}(z) \sum_{i=1}^{m} \frac{\gamma_{ir}^2}{z - \beta_i}.
\end{aligned}$$

This completes the proof. ∎

From Theorem 4.4.1 we obtain

$$\begin{aligned}\lim_{z\to\beta_k}(z-\beta_k)\frac{\Psi_r(T,z)}{\Psi(T,z)} &= \lim_{z\to\beta_k}(z-\beta_k)\sum_{i=1}^{m}\frac{\gamma_{ir}^2}{z-\beta_i}\\ &= \lim_{z\to\beta_k}\gamma_{kr}^2+(z-\beta_k)\sum_{i\neq k}^{m}\frac{\theta_{ir}^2}{z-\beta_i}\\ &= \gamma_{kr}^2\\ &\geq 0.\end{aligned}$$

We also get a non- negative limit. The following theorem presents the relationship of the characteristic polynomial of the Laplacian matrix of a tree T to that of its branches.

Theorem 4.4.2. *Let T be a planted simply generated tree with root r. Suppose $T_1, T_2, \ldots, T_k$ are its branches with $v_1, v_2, \ldots, v_k$ as their roots respectively. Then we have*

$$\frac{\Psi_r(T,z)}{\Psi(T,z)} = \frac{1}{z-1-\sum\limits_{j=1}^{k}\left(\frac{\Psi_{v_j}(T_j,z)}{\Psi(T_j,z)}+1\right)}. \tag{4.39}$$

Proof. Let $G_u \circ H_v$ be a tree obtained by joining the trees G and H by the edge uv. From Proposition 3.3.1 and Theorem 3.3.2 we get that

$$\begin{aligned}\Psi_{L^1(G_u\circ H_v:u)}(z) &= \Psi_{L^1(H:v)}(z)\Psi_{L^1(G:u)}(z) - \Psi_{L^1(H-v:N(v))}(z)\Psi_{L^1(G-u:N(u))}(z)\\ &\quad - \Psi_{L^1(G-u:N(u)\setminus v)}(z)\Psi_{L^1(H:v)}(z).\end{aligned} \tag{4.40}$$

Now, let $G^{(0)}$ be a tree with only one vertex. Suppose we join the root v_1 of the tree T_1 to $G^{(0)}$ to form the tree $G^{(1)}$. Then by equation (4.40) we get

$$\begin{aligned}\Psi_{L^1(G^{(1)}:G^{(0)})}(z) &= (z-1)\Psi_{L^1(T_1:v_1)}(z) - \Psi_{L^1(T_1:v_1)}(z) - \Psi_{L^1(T_1-v_1:N(v_1))}(z)\\ &= \Psi_{L^1(T_1:v_1)}(z)\left(z-2-\frac{\Psi_{L^1(T_1-v_1:N(v_1))}(z)}{\Psi_{L^1(T_1:v_1)}(z)}\right).\end{aligned}$$

Now we construct another tree $G^{(2)}$ by joining the root v_2 of the tree T_2 to the root of the tree $G^{(1)}$. By applying equation (4.40) we get

$$\begin{aligned}\Psi_{L^1(G^{(2)}:G^{(0)})}(z) &= \Psi_{L^1(T_1:v_1)}(z)\Psi_{L^1(T_2:v_2)}(z)\left(z-2-\frac{\Psi_{L^1(T_1-v_1:N(v_1))}(z)}{\Psi_{L^1(T_1:v_1)}(z)}\right)\\ &\quad -\Psi_{L^1(T_1:v_1)}(z)\Psi_{L^1(T_2:v_2)}(z)-\Psi_{L^1(T_1:v_1)}(z)\Psi_{L^1(T_2-v_2:N(v_2))}(z)\\ &= \Psi_{L^1(T_1:v_1)}(z)\Psi_{L^1(T_2:v_2)}(z)\left(z-3-\sum_{i=1}^{k}\frac{\Psi_{L^1(T_i-v_i:N(v_i))}(z)}{\Psi_{L^1(T_i:v_i)}(z)}\right).\end{aligned}$$

Continuous application of equation (4.40) and joining of branches to the root $G^{(0)}$ to form the final tree T gives us equation (4.39). ■

We get the characterisation of a type zero tree from Theorem 4.4.2. Thus, a planted simply generated tree T is a type zero tree if at least one of its branches is a type pole. The proof of this result is similar to that of Theorem 2.6.3. Here we apply Theorem 4.4.2.
Now, if we set

$$H_t(x) = \sum_{\frac{\Psi_r(T,\alpha)}{\Psi(T,\alpha)}=t} W(T)x^{|T|}$$

then we get

$$C_\alpha = \frac{1}{\tau}(H_\infty(\rho) - H_0(\rho))$$

and by the characterisation of a type zero tree we get the functional equation

$$H_0(x) = x\Phi(G(x)) - x\Phi(G(x) - H_\infty(x)).$$

Also, if we set

$$S(z) = \sum_{j=1}^{k}\left(\frac{\Psi_{v_j}(T_j,z)}{\Psi(T_j,z)} + 1\right)$$

then from Theorem 4.4.2 we get that

$$\frac{\Psi_r(T,\alpha)}{\Psi(T,\alpha)} = t$$

for a given eigenvalue α if

$$t = \frac{1}{\alpha - 1 - S(\alpha)},$$

and this gives us the functional equation

$$H_t(x) = \left[y^{\alpha-1-\frac{1}{t}}\right] x\Phi\left(\sum_u H_u(x)y^{u+1}\right), \quad t \neq 0.$$

As for the adjacency spectrum, we can compute the value of C_α for a given α by solving the following system of functional equations;

$$H_0(\rho) = \tau - \rho\Phi(\tau - H_\infty(\rho)), \tag{4.41}$$

$$\sum_{t\neq 0} H_t(\rho)y^{\alpha-1-\frac{1}{t}} = \rho\Phi\left(\sum_{u\geq 0} H_u(\rho)y^{u+1}\right). \tag{4.42}$$

Remark 4.4.3. *One has to resort to computational methods in order to solve this system of functional equations. In particular, one can use Algorithm 4.2.7 but taking into account that at step* 2*Aa the value of t is equal to* $\frac{1}{\alpha-1-u}$.

Knowing how to compute C_α for planted simply generated trees, let us now consider special classes of simply generated trees. For each class we shall state the system of functional equations and results for computing C_1.

4.4.1 Plane trees

The system of functional equations for plane trees is given by

$$H_0\left(\frac{1}{4}\right) = \frac{1}{2} - \frac{1}{2 + 4H_\infty(\frac{1}{4})},$$

$$\sum_{t\neq 0} H_t\left(\frac{1}{4}\right)y^{\alpha-1-\frac{1}{t}} = \frac{1}{4}\sum_{k\geq 0}\left(\sum_{u\geq 0} H_u\left(\frac{1}{4}\right)y^{u+1}\right)^k.$$

and solving them using Algorithm 4.2.7 yields the results shown in Table 4.5 (again, we provide lower and upper bounds).

α	$H_\infty(\frac{1}{4})$	$H_0(\frac{1}{4})$	$\sum_t H_t(\frac{1}{4})$	C_α
1	0.26354000	0.17257773	0.49999273	0.18192454
	0.26354500	0.17257987	0.50000101	0.18193025

Table 4.5: The mean proportion of the eigenvalue 1 in the Laplacian spectrum of a plane tree

This implies that approximately 18.2% of the Laplacian spectrum of a randomly generated large plane tree consist of the eigenvalue 1.

4.4.2 Labelled rooted trees

The following is the system of functional equations for labelled rooted trees:

$$H_0\left(\frac{1}{e}\right) = 1 - e^{-H_\infty\left(\frac{1}{e}\right)},$$
$$\sum_{t\neq 0} H_t\left(\frac{1}{e}\right) y^{\alpha-1-\frac{1}{t}} = \frac{1}{e}\prod_u \left(\sum_{k\geq 0}\frac{1}{k!}H_u\left(\frac{1}{e}\right)^k y^{(u+1)k}\right).$$

By solving this system using Algorithm 4.2.7 we obtain the following results

α	$H_\infty(\frac{1}{e})$	$H_0(\frac{1}{e})$	$\sum_t H_t(\frac{1}{e})$	C_α
1	0.43052500	0.34983233	0.99937221	0.08069267
	0.43125000	0.35030353	1.00099142	0.08094647

Table 4.6: The mean proportion of the eigenvalue 1 in the Laplacian spectrum of a labelled rooted tree

This implies that approximately 8.1% of the Laplacian spectrum of a large labelled rooted tree consist of the eigenvalue 1.

4.4.3 Pruned binary trees

For pruned binary trees, the system of functional equations is as follows

$$H_0\left(\frac{1}{4}\right) = 1 - \frac{1}{4}\left(2 - H_\infty\left(\frac{1}{4}\right)\right)^2,$$
$$\sum_{t\neq 0} H_t\left(\frac{1}{4}\right) y^{\alpha-1-\frac{1}{t}} = \frac{1}{4}\left[1 + \sum_u H_u\left(\frac{1}{4}\right) y^{u+1}\right]^2,$$

and solving them gives us Table 4.7 (we provide lower and upper bounds).

α	$H_\infty(\frac{1}{4})$	$H_0(\frac{1}{4})$	$\sum_t H_t(\frac{1}{4})$	C_α
1	0.36310000	0.33013960	0.99998030	0.03296040
	0.36315000	0.33018052	1.00011017	0.03296948

Table 4.7: The mean proportion of the eigenvalue 1 in the Laplacian spectrum of a large random binary tree

So approximately 3.3% of the Laplacian spectrum of a large pruned binary tree consist of the eigenvalue 1.

Chapter 5

On the distribution of eigenvalues of increasing trees

5.1 Introduction

The main objective of this chapter is to present analogous results to Chapter 4, which was about simply generated generated trees, in the case of increasing trees. In particular, we determine the mean and variance of the distribution of the eigenvalue 0. We also show that the multiplicity of any eigenvalue in the spectra of these trees satisfies a central limit theorem.

5.2 Recursive trees

In this section, we focus on the spectrum of recursive trees. As indicated earlier, recursive trees are increasing trees with the property that they can be constructed by a growth or evolution process. By a growth process, we mean a recursive tree of order 3, for instance, can be constructed by starting with a node (root) labelled 1, then attaching another node (child) with label 2. Now, to attach the last node labelled 3, there are two possible positions, as a child of either 1 or 2. So we have two possible recursive trees of order 3. In general, to add or attach a node labelled n to a recursive tree of order $n-1$, there are exactly $n-1$ possible positions to do so. Using this fact, we can easily deduce that the number of recursive trees of order n, denoted by y_n, is exactly $(n-1)!$.
By marking the root of a recursive tree with the lowest label, a recursive

tree can symbolically be defined by a boxed product. That is, a marked node attached to a set of recursive trees. So we let $Y(x)$ be the exponential generating function, and the symbolic definition translates to the differential equation

$$\frac{dY(x)}{dx} = \exp(Y(x)), \quad \text{where } Y(0) = 0,$$

and this evaluates to

$$Y(x) = \log\left(\frac{1}{1-x}\right).$$

For the purpose of our studies, we define a bivariate exponential generation $Y(x,t)$ as

$$Y(x,u) = \sum_{T\in\mathcal{T}} u^{N_\alpha(T)} \frac{x^{|T|}}{|T|!}$$

where $\mathcal{T}$ is the set of all recursive trees. By treating N_α as an additive parameter and applying Theorem 3.6.3, we get the following result, see also Section 5.4 later.

Corollary 5.2.1. *Let $\mathcal{T}$ be the set of all recursive trees. The mean multiplicity $\mu_\alpha(n)$ of an eigenvalue α in the spectrum of a large random recursive tree of order n is asymptotically given by nC_α where*

$$C_\alpha = \sum_{T\in\mathcal{T}} \frac{(N_\alpha(T) - N_\alpha(T-r))}{(|T|+1)!}. \tag{5.1}$$

In order to compute C_α, we set

$$H_t(x) = \sum_{\frac{\Psi_r(T,\alpha)}{\Psi(T,\alpha)}=t} \frac{x^{|T|+1}}{(|T|+1)!}. \tag{5.2}$$

This implies that

$$Y(x) = \sum_t H_t'(x)$$

and

$$C_\alpha = H_\infty(1) - H_0(1).$$

Based on the classification of trees (see Section 2.6), we get that the value of C_α can be obtained by solving the following system of differential equations;

$$H_0''(x) = \exp(Y(x)) - \exp(H_0'(x)),$$

$$\sum_{t\neq 0} H_t''(x) y^{\alpha-\frac{1}{t}} = \exp\left(\sum_{u\geq 0} H_t'(x) y^u\right).$$

Remark 5.2.2. *Solving this system of differential equations seems very difficult. We have not been able to provide sufficient methods to tackle this problem. However, we shall see later that an explicit solution can be found for the case of the eigenvalue 0.*

5.2.1 The distribution of the eigenvalue 0 in the spectrum of a recursive tree

In this section, we focus on the mean and variance of the multiplicity of the eigenvalue 0 in the spectrum of a large recursive tree.
We first define a bivariate exponential generating function $Y(x,t)$ that takes into account the multiplicities of the eigenvalue 0 and the sizes of recursive trees, as

$$Y(x,t) = \sum_{T \in \mathcal{T}} e^{tN_0(T)} \frac{x^{|T|}}{|T|!},$$

where $\mathcal{T}$ is the set of all recursive trees. As mentioned before, it is known that $Y(x,0)$ satisfies the differential equation

$$\frac{\partial Y(x,0)}{\partial x} = e^{Y(x,0)}, \quad \text{where} \quad Y(0,0) = 0$$

and hence we have

$$Y(x,0) = \log\left(\frac{1}{1-x}\right).$$

We first compute the mean (expectation) and the mean square of the multiplicity of eigenvalue 0. The mean and mean square can be computed from $Y(x,t)$ by considering partial derivatives of $Y(x,t)$ with respect to t and setting $t = 0$. In particular, the coefficient of $\frac{x^n}{n!}$ of the generating function $Y_t(x,0)$, denoted as $n![x^n]Y_t(x,0)$, gives us the total multiplicity of eigenvalue 0 in the spectra of all recursive trees of size n. Since there are $(n-1)!$ recursive trees of size n, the mean number of eigenvalue 0, $\mu_0(n)$, in the spectrum of a random recursive tree is given by

$$\mu_0(n) = n[x^n]Y_t(x,0).$$

Similarly, we can obtain the mean square by considering the coefficients of the second derivative of $Y(x,t)$ with respect to t and setting $t = 0$. Therefore the variance $\sigma^2(n)$ is given by

$$\sigma^2(n) = n[x^n]Y_{tt}(x,0) - (\mu_0(n))^2.$$

Note that

$$Y_t(x,0) = \left.\frac{\partial Y(x,t)}{\partial t}\right|_{t=0} \quad \text{and} \quad Y_{tt}(x,0) = \left.\frac{\partial^2 Y(x,t)}{(\partial t)^2}\right|_{t=0}.$$

We set a generating series $F_w(x,t)$ to be given by

$$F_w(x,t) = \sum_{\frac{\Psi_r(T,0)}{\Psi(T,0)}=w} e^{tN_0(T)} \frac{x^{|T|}}{|T|!}.$$

Hence we have that

$$Y(x,t) = F_0(x,t) + F_\infty(x,t).$$

Based on the classification of the various types of rooted trees (see Theorem 2.6.3 in Section 2.6 and Theorem 4.3.1 in Section 4.3), we get the following differential equations;

$$\frac{\partial F_\infty(x,t)}{\partial x} = e^t e^{F_0(x,t)}, \tag{5.3}$$

$$\frac{\partial F_0(x,t)}{\partial x} = e^{-t}\left(e^{F_0(x,t)+F_\infty(x,t)} - e^{F_0(x,t)}\right). \tag{5.4}$$

Now, we compute the derivatives of equations (5.3) and (5.4) with respect to t and set $t = 0$. For the sake of simplicity, we let

$$G_w(x,0) = \left.\frac{\partial F_w(x,t)}{\partial t}\right|_{t=0}.$$

We get

$$\frac{\partial G_\infty(x,0)}{\partial x} = e^{F_0(x,0)} + G_0(x,0)e^{F_0(x,0)}, \tag{5.5}$$

$$\frac{\partial G_0(x,0)}{\partial x} = e^{F_0(x,0)+F_\infty(x,0)}(G_0(x,0) + G_\infty(x,0) - 1) + e^{F_0(x,0)}(1 - G_0(x,0)). \tag{5.6}$$

Note that

$$Y_t(x,0) = G_0(x,0) + G_\infty(x,0)$$

and

$$Y(x,0) = F_0(x,0) + F_\infty(x,0) = \log\left(\frac{1}{1-x}\right). \tag{5.7}$$

We can obtain the mean by analysing the coefficients of the generating function $Y_t(x,0)$, which we get from solving the differential equation obtained by summing the equations (5.5) and (5.6). Thus solving the differential equation

$$\frac{\partial Y_t(x,0)}{\partial x} = \frac{1}{1-x}(Y_t(x,0)-1) + 2e^{F_0(x,0)}. \tag{5.8}$$

Before we can proceed to solve the differential equation (5.8), we need to first solve for $F_0(x,0)$. From equations (5.3) and (5.4) we get

$$\frac{\partial F_\infty(x,0)}{\partial x} = e^{Y(x,0)-F_\infty(x,0)}, \quad F_\infty(0,0) = 0, \tag{5.9}$$

$$\frac{\partial F_0(x,0)}{\partial x} = e^{Y(x,0)} - F_\infty(x,0), \quad F_0(0,0) = 0. \tag{5.10}$$

Let us consider the differential equation (5.9) and simplify to get

$$\begin{aligned} \frac{\partial F_\infty(x,0)}{\partial x} &= \frac{e^{-F_\infty(x,0)}}{1-x} \\ e^{F_\infty(x,0)} &= \int \frac{1}{1-x}dx \\ &= -\log(1-x) + C \end{aligned}$$

where the constant $C = 1$ is obtained by using the initial condition $F_\infty(0,0) = 0$. This gives us

$$F_\infty(x,0) = \log(1-\log(1-x))$$

and substituting into equation (5.7) yields

$$F_0(x,0) = -\log[(1-x)(1-\log(1-x))].$$

Now, let us go back to solve the differential equation (5.8). We have

$$\begin{aligned} \frac{\partial Y_t(x,0)}{\partial x} &= \frac{1}{1-x}(Y_t(x,0)-1) + \frac{2}{(1-x)(1-\log(1-x))} \\ \frac{\partial Y_t(x,0)}{\partial x} - \frac{1}{1-x}Y_t(x,0) &= \frac{1}{1-x}\left(\frac{1+\log(1-x)}{1-\log(1-x)}\right). \end{aligned}$$

Using the integrating factor

$$e^{-\int \frac{1}{1-x}dx} = 1-x$$

we get

$$\begin{aligned}(1-x)Y_t(x,0) &= \int_0^x \frac{1+\log(1-w)}{1-\log(1-w)}dw\\ Y_t(x,0) &= \frac{1}{1-x}\int_0^x \frac{1+\log(1-w)}{1-\log(1-w)}dw.\end{aligned}$$

We wish to find the asymptotic behaviour of $[x^n]Y_t(x,0)$. This is derived as follows;

$$\begin{aligned}Y_t(x,0) &= \frac{1}{1-x}\int_0^x \frac{1+\log(1-w)}{1-\log(1-w)}dw\\ &= \frac{1}{1-x}\int_{1-x}^1 \frac{1+\log(u)}{1-\log(u)}du\\ &= \frac{1}{1-x}\left(\int_0^1 \frac{1+\log(u)}{1-\log(u)}du - \int_0^{1-x} \frac{1+\log(u)}{1-\log(u)}du\right)\\ &= \frac{1}{1-x}\left(2G-1+\int_0^{1-x}\left(1-\frac{2}{1-\log(u)}\right)du\right)\\ &= \frac{2G-1}{1-x}+1-\frac{1}{1-x}\int_0^{1-x}\frac{2}{1-\log(u)}du\\ &= \frac{2G-1}{1-x}+1+\mathcal{O}\left(\left|\frac{1}{\log(1-x)}\right|\right),\end{aligned}$$

where G is the Euler-Gompertz constant. Therefore by singularity analysis (see Section 2.5), we get

$$[x^n]Y_t(x,0) = 2G-1+\mathcal{O}\left(\frac{1}{n\log^2(n)}\right).$$

Therefore, the limiting mean multiplicity of the eigenvalue 0 is approximately

$$(2G-1)n+\mathcal{O}\left(\frac{1}{\log^2(n)}\right).$$

Since $2G-1 = 0.19269473$, we infer that approximately 19.3% of the spectrum of a large random recursive tree consist of the eigenvalue 0.

Since our next goal is to compute the variance, let us proceed to compute the mean square of the multiplicities of the eigenvalue 0. Here, we consider the second partial derivative of the differential equations (5.3) and (5.4) with respect to t and set $t=0$. For the sake of simplicity, we let

$$H_w(x,0) = \left.\frac{\partial^2 F_w(x,t)}{(\partial t)^2}\right|_{t=0}.$$

This gives us

$$\begin{aligned}\frac{\partial H_\infty(x,0)}{\partial x} &= e^{F_0(x,0)}(1+2G_0(x,0)+G_0(x,0)^2)+e^{F_0(x,0)}H_\infty(x,0)\\ &= e^{F_0(x,0)}(1+G_0(x,0))^2+e^{F_0(x,0)}H_0(x,0) \end{aligned} \tag{5.11}$$

and

$$\begin{aligned}\frac{\partial H_0(x,0)}{\partial x} = {}& e^{F_\infty(x,0)+F_0(x,0)}(1-G_0(x,0)-G_\infty(x,0))^2\\ &+e^{F_\infty(x,0)+F_0(x,0)}(H_0(x,0)+H_\infty(x,0))\\ &-e^{F_0(x,0)}(1-G_0(x,0))^2-e^{F_0(x,0)}H_0(x,0). \end{aligned} \tag{5.12}$$

Summing them and simplifying yields

$$\begin{aligned}\frac{\partial Y_{tt}(x,0)}{\partial x} &= e^{Y(x,0)}(1-Y_t(x,0))^2+e^{Y(x,0)}Y_{tt}(x,0)+4e^{F_0(x,0)}G_0(x,0)\\ &= \frac{(1-Y_t(x,0))^2}{1-x}+\frac{Y_{tt}(x,0)}{1-x}+\frac{4G_0(x,0)}{(1-x)(1-\log(1-x))}. \end{aligned} \tag{5.13}$$

Let us first compute $G_0(x,0)$ from the differential equation (5.6). We have

$$\begin{aligned}\frac{\partial G_0(x,0)}{\partial x}+\frac{G_0(x,0)}{(1-x)(1-\log(1-x))} &= \frac{\log(1-x)}{(1-x)(1-\log(1-x))}\\ &\quad+\frac{1}{(1-x)^2}\int_0^x\frac{1+\log(1-w)}{1-\log(1-w)}dw. \end{aligned}$$

Using the integrating factor

$$\exp\left(\int\frac{1}{(1-x)(1-\log(1-x))}dx\right)=1-\log(1-x)$$

we get

$$\begin{aligned}(1-\log(1-x))G_0(x,0) = \int_0^x\Bigg(&\frac{\log(1-u)}{1-u}\\ &+\frac{1-\log(1-u)}{(1-u)^2}\int_0^u\frac{1+\log(1-w)}{1-\log(1-w)}dw\Bigg)\,du, \end{aligned}$$

so

$$G_0(x,0) = \frac{1}{1-\log(1-x)}\left[\int_0^x \left(\frac{\log(1-u)}{1-u} + \frac{1-\log(1-u)}{(1-u)^2}\int_0^u \frac{1+\log(1-w)}{1-\log(1-w)}dw\right) du\right].$$

Now let us go back to solve for $Y_{tt}(x,0)$ in the differential equation (5.13). We have

$$\frac{\partial Y_{tt}(x,0)}{\partial x} - \frac{Y_{tt}(x,0)}{1-x} = \frac{(1-Y_t(x,0))^2}{1-x} + \frac{4G_0(x,0)}{(1-x)(1-\log(1-x))},$$

and using the integrating factor

$$e^{-\int \frac{1}{1-x}dx} = 1-x$$

we get

$$(1-x)Y_{tt}(x,0) = \int_0^x \left((1-Y_t(u,0))^2 + \frac{4G_0(u,0)}{(1-\log(1-u))}\right) du$$

and hence

$$Y_{tt}(x,0) = \frac{1}{1-x}\left[\int_0^x \left((1-Y_t(u,0))^2 + \frac{4G_0(u,0)}{(1-\log(1-u))}\right) du\right].$$

We now need to consider the asymptotic behaviour of $[x^n]Y_{tt}(x,0)$. We first consider that of $G_0(x,0)$. Note that

$$\int_0^u \frac{1+\log(1-w)}{1-\log(1-w)}dw = 2G - 1 + \mathcal{O}(|1-u|)$$

and

$$\int_0^x \frac{\log(1-u)}{1-u}du = -\frac{1}{2}\log^2(1-x).$$

So

$$\begin{aligned} G_0(x,0) &= \frac{1}{1-\log(1-x)}\left[-\frac{1}{2}\log^2(1-x) + (2G-1)\int_0^x \frac{1-\log(1-u)}{(1-u)^2} + \mathcal{O}\left(\int_0^x \left|\frac{\log(1-u)}{1-u}\right| du\right)\right] \\ &= \frac{2G-1}{1-x} + \mathcal{O}\left(\frac{1}{|(1-x)\log(1-x)|}\right). \end{aligned}$$

Therefore we get

$$(1-Y_t(u,0))^2+\frac{4G_0(u,0)}{(1-\log(1-u))}=\frac{(2G-1)^2}{(1-u)^2}+\mathcal{O}\left(\frac{1}{(1-u)\log^2(1-u)}\right)$$

and it follows that the integral

$$\int_0^1\left((1-Y_t(u,0))^2+\frac{4G_0(u,0)}{(1-\log(1-u))}-\frac{(2G-1)^2}{(1-u)^2}\right)du$$

converges. So we infer that

$$\begin{aligned}
Y_{tt}(x,0)&=\frac{(2G-1)^2x}{(1-x)^2}\\
&\quad+\frac{1}{1-x}\int_0^1\left((1-Y_t(u,0))^2+\frac{4G_0(u,0)}{(1-\log(1-u))}-\frac{(2G-1)^2}{(1-u)^2}\right)du\\
&\quad-\frac{1}{1-x}\int_x^1\left((1-Y_t(u,0))^2+\frac{4G_0(u,0)}{(1-\log(1-u))}-\frac{(2G-1)^2}{(1-u)^2}\right)du\\
&=\frac{(2G-1)^2x}{(1-x)^2}+\frac{K}{1-x}+\mathcal{O}\left(\frac{1}{|(1-x)\log(1-x)|}\right),
\end{aligned}$$

where K is given by the integral

$$\int_0^1\left((1-Y_t(u,0))^2+\frac{4G_0(u,0)}{(1-\log(1-u))}-\frac{(2G-1)^2}{(1-u)^2}\right)du.$$

By singularity analysis, we get

$$[x^n]Y_{tt}(x,0)=(2G-1)^2n+K+\mathcal{O}\left(\frac{1}{\log^2(n)}\right).$$

Finally, the variance is given by

$$\sigma^2(n)=Kn+\mathcal{O}\left(\frac{n}{\log^2(n)}\right).$$

The constant K can be simplified and evaluated numerically:

$$\begin{aligned}
K&=\int_0^1\left((1-Y_t(u,0))^2+\frac{4G_0(u,0)}{(1-\log(1-u))}-\frac{(2G-1)^2}{(1-u)^2}\right)du\\
&=4(G^2-G)+8\int_0^1\frac{\log(1-\log w)}{(1-\log w)^2}dw\\
&\approx 0.138629278.
\end{aligned}$$

So the variance is approximately $0.138629278n$.

5.3 Binary increasing trees

A binary increasing tree has the property that each vertex has 2 possible places to which a child can be attached, that is, a left or right child. In view of that, to attach a node labelled n to an existing binary increasing tree of order $n-1$, there are n possible places to do so. Therefore, if we let y_n be the number of binary increasing trees of order n, then we have that

$$b_n = \prod_{j=1}^{n-1}(j+1) = n!.$$

Let $\mathbb{T}$ be the set of all binary increasing trees. We let the exponential generating function $B(x)$ of binary increasing trees be given by

$$B(x) = \sum_{T\in\mathbb{T}} \frac{x^{|T|}}{|T|!} = \sum_{n\geq 1} b_n \frac{x^n}{n!} = \sum_{n\geq 1} x^n = \frac{x}{1-x}.$$

Also, $B(x)$ satisfies

$$\frac{dB(x)}{dx} = \sum_{T\in\mathbb{T}} \frac{x^{|T|-1}}{(|T|-1)!} = (1+B(x))^2, \quad B(0) = 0.$$

We include another variable u in our generating function to mark the multiplicities of eigenvalues. Thus,

$$B(x,u) = \sum_{T\in\mathbb{T}} u^{N_\alpha(T)} \frac{x^{|T|}}{|T|!}.$$

Further, we treat N_α as an additive parameter and apply Theorem 3.6.3 to get the following result, see also Section 5.4 later.

Corollary 5.3.1. *Let $\mathbb{T}$ be the set of all binary increasing trees. The mean multiplicity $\mu_\alpha(n)$ of an eigenvalue α in the spectrum of a large random binary increasing tree of order n is asymptotically given by $C_\alpha(n+1)$, where*

$$C_\alpha = 2\sum_{T\in\mathbb{T}} \frac{(N_\alpha(T) - N_\alpha(T-r))}{(|T|+2)!}. \tag{5.14}$$

We now focus on C_α and set

$$H_t(x) = \sum_{\frac{\Psi_r(T,\alpha)}{\Psi(T,\alpha)}=t} \frac{x^{|T|+2}}{(|T|+2)!}. \tag{5.15}$$

This implies that

$$B(x) = \sum_t H_t''(x)$$

and

$$C_\alpha = 2\Big(H_\infty(1) - H_0(1)\Big).$$

Based on the characterisation of rooted trees (see Theorem 2.6.3 in Section 2.6 and Theorem 4.3.1 in Section 4.3), we get that the value of C_α can be obtained by solving the following system of differential equations;

$$H_0'''(x) = \Big(1 + B(x)\Big)^2 - \Big(1 + H_0''(x)\Big)^2,$$

$$\sum_{t \neq 0} H_t'''(x) y^{\alpha - \frac{1}{t}} = \left(1 + \sum_{u \geq 0} H_t''(x) y^u\right)^2.$$

Remark 5.3.2. *Here, we do not provide an algorithm to solve this system. However, we shall provide a solution to this system for the case of the eigenvalue 0.*

5.3.1 The distribution of the eigenvalue 0 in the spectrum of a binary increasing tree

Our goal here is to determine the mean and variance for the multiplicity of the eigenvalue 0 in the spectra of binary trees. With this, we let $N_0(T)$ denote the multiplicity of the eigenvalue 0 in the spectrum of a binary increasing tree T and define a bivariate exponential generating function $B(x,u)$ that takes into account the multiplicities of the eigenvalue 0 and the sizes of binary increasing trees, as

$$B(x,u) = \sum_{T \in \mathbb{T}} u^{N_0(T)} \frac{x^{|T|}}{|T|!}.$$

The mean and mean square can be computed from $B(x,u)$ by considering partial derivatives of $B(x,u)$ with respect to u and setting $u = 1$. In particular, the coefficient of $\frac{x^n}{n!}$ of the generating function $B_u(x,1)$, denoted as $n![x^n]B_u(x,1)$, gives us the total multiplicity of eigenvalue 0 in the spectra of all binary increasing trees of size n. Since there are $n!$ binary increasing trees of size n, the mean multiplicity of eigenvalue 0, $\mu_0(n)$, in the spectrum of a binary increasing tree is given by

$$\mu_0(n) = [x^n]B_u(x,1).$$

Similarly, we can obtain the mean square by considering the coefficients of the second derivative of $Y(x,u)$ with respect to u and setting $u = 1$. The variance $\sigma^2(n)$ is given by

$$\sigma^2(n) = [x^n]B_{uu}(x,1) + [x^n]B_u(x,1) - ([x^n]B_u(x,1))^2.$$

Note that

$$B_u(x,1) = \left.\frac{\partial B(x,u)}{\partial u}\right|_{u=1} \quad \text{and} \quad B_{uu}(x,1) = \left.\frac{\partial^2 B(x,u)}{(\partial u)^2}\right|_{u=1}.$$

We set a generating series $F_w(x,u)$ to be given by

$$F_w(x,u) = \sum_{\frac{\Psi_r(T,0)}{\Psi(T,0)}=w} u^{N_0(T)} \frac{x^{|T|}}{|T|!}.$$

Hence we have that

$$B(x,u) = F_0(x,u) + F_\infty(x,u).$$

Based on the characterisation of the various types of trees, we get the following differential equations;

$$\frac{\partial F_\infty(x,u)}{\partial x} = u + 2uF_0(x,u) + uF_0(x,u)^2, \tag{5.16}$$

$$\frac{\partial F_0(x,u)}{\partial x} = 2u^{-1}B(x,u) + u^{-1}B(x,u)^2 - 2u^{-1}F_0(x,u) - u^{-1}F_0(x,u)^2. \tag{5.17}$$

Now, we compute the derivatives of equations (5.16) and (5.17) with respect to u and set $u = 1$. For the sake of simplicity, we let

$$G_w(x,1) = \left.\frac{\partial F_w(x,u)}{\partial u}\right|_{u=1} \quad \text{and} \quad H_w(x,1) = \left.\frac{\partial^2 F_w(x,u)}{(\partial u)^2}\right|_{u=1}.$$

We get

$$\begin{aligned}
\frac{\partial G_\infty(x,1)}{\partial x} &= 1 + 2F_0(x,1) + F_0(x,1)^2 + 2G_0(x,1) + 2G_0(x,1)F_0(x,1), \\
\frac{\partial H_\infty(x,1)}{\partial x} &= 4G_0(x,1) + 2G_0(x,1)^2 + 4G_0(x,1)F_0(x,1) + 2H_0(x,1) \\
&\quad + 2H_0(x,1)F_0(x,1),
\end{aligned}$$

and

$$\begin{aligned}\frac{\partial G_0(x,1)}{\partial x} &= 2B_u(x,1)\Big[1+B(x,1)\Big] - B(x,1)\Big[2+B(x,1)\Big]\\ &\quad + F_0(x,1)\Big[2+F_0(x,1)\Big] - 2G_0(x,1)\Big[1+F_0(x,1)\Big],\\ \frac{\partial H_0(x,1)}{\partial x} &= 2B(x,1)\Big[2+B(x,1)\Big] - 2B_u(x,1)\Big[2+2B(x,1)-B_u(x,1)\Big]\\ &\quad + 2B_{uu}(x,1)\Big[1+B(x,1)\Big] - 2F_0(x,1)\Big[2+F_0(x,1)\Big]\\ &\quad + 2G_0(x,1)\Big[2+2F_0(x,1)-G_0(x,1)\Big] - 2H_0(x,1)\Big[1+F_0(x,1)\Big].\end{aligned}$$

Recall that

$$B(x) = B(x,1) = \frac{x}{1-x}.$$

Now, computing the first moment, we have

$$\begin{aligned}\frac{\partial B_u(x,1)}{\partial x} &= \frac{\partial G_0(x,1)}{\partial x} + \frac{\partial G_\infty(x,1)}{\partial x}\\ &= 2F_0(x,1)\Big[2+F_0(x,1)\Big] + \frac{1-4x+2x^2}{(1-x)^2} + \frac{2}{1-x}B_u(x,1).\end{aligned}$$

Using the integrating factor

$$\exp\left(-2\int \frac{1}{1-x}dx\right) = (1-x)^2$$

we get

$$B_u(x,1) = \frac{1}{(1-x)^2}\int_0^x \left(1-4t+2t^2+2(1-t)^2F_0(t,1)\Big[2+F_0(t,1)\Big]\right)dt.$$

Now, let us compute $F_0(t,1)$. To do this, we first compute $F_\infty(x,1)$ from equation (5.16) and use the fact that

$$F_0(t,1) = B(x,1) - F_\infty(x,1).$$

Thus, we get a Riccati equation,

$$\frac{dF_\infty(x,1)}{dx} = \frac{1}{(1-x)^2} - \frac{2F_\infty(x,1)}{1-x} + F_\infty(x,1)^2. \tag{5.18}$$

We let $y(x) = \frac{A}{1-x}$ be a particular solution of the differential equation (5.18) and simplify to get $A = \frac{3-\sqrt{5}}{2}$. So if we let

$$F_\infty(x,1) = y(x) + \frac{1}{z(x)}$$

then we get

$$\frac{dz(x)}{dx} = -\left(\frac{1-\sqrt{5}}{1-x}\right) z(x) - 1$$

and using the integrating factor

$$\exp\left(\int \frac{1-\sqrt{5}}{1-x} dx\right) = (1-x)^{\sqrt{5}-1}$$

we get

$$z = \frac{(1-x)^{\sqrt{5}} + c\sqrt{5}}{\sqrt{5}(1-x)^{\sqrt{5}-1}}.$$

Therefore, we have that

$$F_\infty(x,1) = \frac{3-\sqrt{5}}{2(1-x)} + \frac{\sqrt{5}(1-x)^{\sqrt{5}-1}}{(1-x)^{\sqrt{5}} + c\sqrt{5}}.$$

Since $F_\infty(0,1) = 0$ we get $c = \frac{(3+\sqrt{5})^2}{-4\sqrt{5}}$.
So we finally have

$$F_\infty(x,1) = \frac{3-\sqrt{5}}{2(1-x)} + \frac{4\sqrt{5}(1-x)^{\sqrt{5}-1}}{4(1-x)^{\sqrt{5}} - (3+\sqrt{5})^2}$$

and hence

$$F_0(x,1) = \frac{x}{1-x} - \frac{3-\sqrt{5}}{2(1-x)} - \frac{4\sqrt{5}(1-x)^{\sqrt{5}-1}}{4(1-x)^{\sqrt{5}} - (3+\sqrt{5})^2}.$$

Now, substituting $F_0(x,1)$ into $B_u(x,1)$ yields

$$B_u(x,1) = \frac{1}{(1-x)^2} \int_0^x \left(2 - \sqrt{5} + \frac{160(1-t)^{2\sqrt{5}}}{\left[4(1-t)^{\sqrt{5}} - 14 - 6\sqrt{5}\right]^2} + \frac{\left[8\sqrt{5} - 40\right](1-t)^{\sqrt{5}}}{4(1-t)^{\sqrt{5}} - 14 - 6\sqrt{5}}\right) dt.$$

Let us now determine the asymptotic behaviour of $[x^n]B_u(x,1)$. We have

$$\begin{aligned}
B_u(x,1) &= \frac{1}{(1-x)^2}\int_{1-x}^{0}\left(2-\sqrt{5}+\frac{160(w)^{2\sqrt{5}}}{\left[4(w)^{\sqrt{5}}-14-6\sqrt{5}\right]^2}\right.\\
&\quad\left.+\frac{\left[8\sqrt{5}-40\right](w)^{\sqrt{5}}}{4(w)^{\sqrt{5}}-14-6\sqrt{5}}\right)dw\\
&= \frac{1}{(1-x)^2}\int_{0}^{1}\left(2-\sqrt{5}+\frac{160(w)^{2\sqrt{5}}}{\left[4(w)^{\sqrt{5}}-14-6\sqrt{5}\right]^2}\right.\\
&\quad\left.+\frac{\left[8\sqrt{5}-40\right](w)^{\sqrt{5}}}{4(w)^{\sqrt{5}}-14-6\sqrt{5}}\right)dw\\
&\quad-\frac{1}{(1-x)^2}\int_{0}^{1-x}\left(2-\sqrt{5}+\frac{160(w)^{2\sqrt{5}}}{\left[4(w)^{\sqrt{5}}-14-6\sqrt{5}\right]^2}\right.\\
&\quad\left.+\frac{\left[8\sqrt{5}-40\right](w)^{\sqrt{5}}}{4(w)^{\sqrt{5}}-14-6\sqrt{5}}\right)dw\\
&= \frac{1}{(1-x)^2}\int_{0}^{1}\left(2-\sqrt{5}+\frac{160(w)^{2\sqrt{5}}}{\left[4(w)^{\sqrt{5}}-14-6\sqrt{5}\right]^2}\right.\\
&\quad\left.+\frac{\left[8\sqrt{5}-40\right](w)^{\sqrt{5}}}{4(w)^{\sqrt{5}}-14-6\sqrt{5}}\right)dw\\
&\quad-\frac{1}{(1-x)^2}\int_{0}^{1-x}\left[2-\sqrt{5}+\mathcal{O}\left(w^{\sqrt{5}}\right)\right]dw\\
&= \frac{C}{(1-x)^2}+\frac{\sqrt{5}-2}{1-x}+\mathcal{O}\left((1-x)^{\sqrt{5}-1}\right),
\end{aligned}$$

where

$$C=\int_0^1\left(2-\sqrt{5}+\frac{160(w)^{2\sqrt{5}}}{\left[4(w)^{\sqrt{5}}-14-6\sqrt{5}\right]^2}+\frac{\left[8\sqrt{5}-40\right](w)^{\sqrt{5}}}{4(w)^{\sqrt{5}}-14-6\sqrt{5}}\right)dw.$$

By singularity analysis we get

$$\begin{aligned}\mu_0(n) &= [x^n]B_u(x,1)\\ &= C(n+1) + \sqrt{5} - 2 + \mathcal{O}(n^{-\sqrt{5}}).\end{aligned}$$

Since $C = 0.0857526$, we infer that on average approximately 8.6% of the spectrum of a large binary increasing tree consist of the eigenvalue 0.
Now let us compute the second moment. Here, we have

$$\begin{aligned}\frac{\partial B_{uu}(x,1)}{\partial x} &= \frac{\partial H_0(x,1)}{\partial x} + \frac{\partial H_\infty(x,1)}{\partial x}\\ &= \frac{4x}{1-x} + \frac{2x^2}{(1-x)^2} - \frac{4B_u(x,1)}{1-x} + 2B_u(x,1)^2 + \frac{2B_{uu}(x,1)}{1-x}\\ &\quad - 4F_0(x,1) - 2F_0(x,1)^2 + 8F_0(x,1)G_0(x,1) + 8G_0(x,1).\end{aligned}$$

Using the integrating factor

$$\exp\left(2\int \frac{1}{1-x}\mathrm{d}x\right) = (1-x)^2,$$

we get

$$\begin{aligned}B_{uu}(x,1) &= \frac{1}{(1-x)^2}\int_0^x \Big(4t - 2t^2 - 4(1-t)B_u(t,1) + 2(1-t)^2Bu(t,1)^2\\ &\quad - 4(1-t)^2F_0(t,1) - 2(1-t)^2F_0(t,1)^2\\ &\quad +8(1-t)^2G_0(t,1)\Big[F_0(t,1)+1\Big]\Big)\,\mathrm{d}t.\\ &= \frac{1}{(1-x)^2}\int_0^x 2\Big[(1-t)B_u(t,1) - 1\Big]^2 - 2(1-t)^2\Big[F_0(t,1)+1\Big]^2\\ &\quad + 8(1-t)^2\Big[F_0(t,1)+1\Big]G_0(t,1)\,\mathrm{d}t.\end{aligned} \tag{5.19}$$

Now, we need to compute $G_0(x,1)$. Here, we have

$$\frac{\partial G_0(x,1)}{\partial x} = \frac{2}{1-x}B_u(x,1) - \frac{1}{(1-x)^2} + \Big[F_0(x,1)+1\Big]^2 - 2G_0(x,1)\Big[F_0(x,1)+1\Big].$$

Using the integrating factor

$$\exp\left(2\int \Big[F_0(x,1)+1\Big]dx\right) = \Big[2(1-x)^{\sqrt{5}} - 7 - 3\sqrt{5}\Big]^2(1-x)^{1-\sqrt{5}}$$

we get

$$
\begin{aligned}
G_0(x,1) &= \frac{(1-x)^{\sqrt{5}-1}}{\left[2(1-x)^{\sqrt{5}}-7-3\sqrt{5}\right]^2}\int_0^x \left[\frac{-\left[2(1-t)^{\sqrt{5}}-7-3\sqrt{5}\right]^2}{(1-t)^{1+\sqrt{5}}}\right.\\
&\quad+\frac{2\left[2(1-t)^{\sqrt{5}}-7-3\sqrt{5}\right]^2}{(1-t)^{\sqrt{5}}}B_u(t,1)\\
&\quad\left.+\frac{\left[2(1-t)^{\sqrt{5}}-7-3\sqrt{5}\right]^2\Big(F_0(t,1)+1\Big)^2}{(1-t)^{\sqrt{5}-1}}\right]dt\\
&= \frac{(1-x)^{\sqrt{5}-1}}{\left[2(1-x)^{\sqrt{5}}-7-3\sqrt{5}\right]^2}\int_0^x \left[\frac{8(7+3\sqrt{5})}{1-t}-\frac{2(29+13\sqrt{5})}{(1-t)^{1+\sqrt{5}}}\right.\\
&\quad\left.+\frac{2(1+\sqrt{5})}{(1-t)^{1-\sqrt{5}}}+\frac{2\left[2(1-t)^{\sqrt{5}}-7-3\sqrt{5}\right]^2}{(1-t)^{\sqrt{5}}}B_u(t,1)\right]dt.
\end{aligned}
$$

We have that

$$
\begin{aligned}
&\int_0^x \left[\frac{8(7+3\sqrt{5})}{1-t}-\frac{2(29+13\sqrt{5})}{(1-t)^{1+\sqrt{5}}}+\frac{2(1+\sqrt{5})}{(1-t)^{1-\sqrt{5}}}\right]dt\\
&= -8(7+3\sqrt{5})\log(1-x)-\frac{2(29+13\sqrt{5})(1-x)^{-\sqrt{5}}}{\sqrt{5}}\\
&\quad-\frac{2(1+\sqrt{5})(1-x)^{\sqrt{5}}}{\sqrt{5}}+8(7+3\sqrt{5})\\
&= -\frac{2(29+13\sqrt{5})(1-x)^{-\sqrt{5}}}{\sqrt{5}}+\mathcal{O}\Big(\log(1-x)\Big).
\end{aligned}
$$

From what we know about $B_u(t,1)$, we also have that

$$
\begin{aligned}
&\int_0^x \frac{2\left[2(1-t)^{\sqrt{5}}-7-3\sqrt{5}\right]^2}{(1-t)^{\sqrt{5}}}B_u(t,1)dt\\
&= \int_0^x \frac{2\left[2(1-t)^{\sqrt{5}}-7-3\sqrt{5}\right]^2}{(1-t)^{\sqrt{5}+2}}\left[C+(\sqrt{5}-2)(1-t)+\mathcal{O}\Big((1-t)^{\sqrt{5}+1}\Big)\right]dt\\
&= \frac{2C(29+13\sqrt{5})}{(1-x)^{\sqrt{5}+1}}+\frac{100+44\sqrt{5}}{5(1-x)^{\sqrt{5}}}+\mathcal{O}\Big((1-x)^{-\sqrt{5}}\Big).
\end{aligned}
$$

From the expansion

$$\left[2(1-x)^{\sqrt{5}}-7-3\sqrt{5}\right]^{-2}=\frac{1}{(7+3\sqrt{5})^2}+\mathcal{O}\left((1-x)^{\sqrt{5}}\right),$$

we get

$$G_0(x,1)=\frac{C(\sqrt{5}-1)}{2(1-x)^2}+\frac{15-7\sqrt{5}}{10(1-x)}+\mathcal{O}(1).$$

Since we are interested in the asymptotic behaviour of $[x^n]B_{uu}(x,1)$, let us consider the following functions. We know that

$$\begin{aligned}2\left[(1-t)B_u(t,1)-1\right]^2&=2\left[\frac{C}{1-t}+\sqrt{5}-3+\mathcal{O}\left((1-t)^{\sqrt{5}}\right)\right]^2\\&=\frac{2C^2}{(1-t)^2}+\frac{4C(\sqrt{5}-3)}{1-t}+28-12\sqrt{5}+\mathcal{O}\left((1-t)^{\sqrt{5}-1}\right).\end{aligned}$$

Also, $8(1-t)^2\left[F_0(t,1)+1\right]G_0(t,1)$ evaluates to

$$\begin{aligned}&=\left[4(\sqrt{5}-1)(1-t)-\frac{32\sqrt{5}(1-t)^{\sqrt{5}+1}}{4(1-t)^{\sqrt{5}}-14-6\sqrt{5}}\right]\left[\frac{C(\sqrt{5}-1)}{2(1-t)^2}+\frac{15-7\sqrt{5}}{10(1-t)}+\mathcal{O}(1)\right]\\&=-\frac{4C(\sqrt{5}-3)}{1-t}+\mathcal{O}(1)\end{aligned}$$

and $-2(1-t)^2\left[F_0(t,1)+1\right]^2$ evaluates to

$$\begin{aligned}&=-2\left[\frac{\sqrt{5}-1}{2}-\frac{4\sqrt{5}(1-t)^{\sqrt{5}}}{4(1-t)^{\sqrt{5}}-14-6\sqrt{5}}\right]^2\\&=\sqrt{5}-3+\frac{(40-8\sqrt{5})(1-t)^{\sqrt{5}}}{4(1-t)^{\sqrt{5}}-14-6\sqrt{5}}-\frac{160(1-t)^{2\sqrt{5}}}{\left[4(1-t)^{\sqrt{5}}-14-6\sqrt{5}\right]^2}\\&=\mathcal{O}(1).\end{aligned}$$

For the sake of simplicity, we set

$$B_{uu}(x,1)=\frac{1}{(1-x)^2}\int_0^x f(t)dt$$

where $f(t)$ is as in equation (5.19).

So combining the earlier results, we get

$$f(t) = \frac{2C^2}{(1-t)^2} + \mathcal{O}(1)$$

and this implies that

$$A = \int_0^1 \left(f(t) - \frac{2C^2}{(1-t)^2} \right) dt$$

converges. Therefore, we get

$$\begin{aligned} B_{uu}(x,1) &= \frac{2C^2}{(1-x)^3} + \frac{1}{(1-x)^2} \int_0^1 \left(f(t) - \frac{2C^2}{(1-t)^2} \right) dt \\ &\quad - \frac{1}{(1-x)^2} \int_x^1 \left(f(t) - \frac{2C^2}{(1-t)^2} \right) dt \\ &= \frac{2C^2}{(1-x)^3} + \frac{A}{(1-x)^2} + \mathcal{O}\left(\frac{1}{1-x} \right). \end{aligned}$$

By singularity analysis we have that

$$[x^n]B_{uu}(x,1) = C^2(n^2+3n+2) + A(n+1) + \mathcal{O}(1).$$

So the variance is

$$\begin{aligned} \sigma^2(n) &= C^2(n^2+3n+2) + A(n+1) + \mathcal{O}(1) + C(n+1) + \sqrt{5} - 2 + \mathcal{O}(n^{-\sqrt{5}}) \\ &\quad - \left(C(n+1) + \sqrt{5} - 2 + \mathcal{O}(n^{-\sqrt{5}}) \right)^2 \\ &= \left[C^2 + C(5 - 2\sqrt{5}) + A \right] n + \mathcal{O}(1). \end{aligned}$$

By means of numerical approximation, we find that

$$\begin{aligned} A &= \int_0^1 \left(f(t) - \frac{2C^2}{(1-t)^2} \right) dt \\ &\approx 0.019250. \end{aligned}$$

Hence the variance is

$$\sigma^2(n) = 0.030485n + \mathcal{O}(1).$$

5.4 Limiting distribution of eigenvalues in increasing trees

In this section, we focus on the limiting distribution of eigenvalues in the spectra of recursive trees and binary increasing trees. We first introduce some notations.

We let $\mathcal{N}(0,1)$ denote the standard normal distribution and let $\xrightarrow{d}$ denote convergence in distribution. We let $\mathbb{T}_n$ and $\mathcal{T}_n$ denote uniform random binary increasing trees and recursive trees of order n respectively.

In order to show convergence of the distribution of eigenvalues in the spectrum of binary increasing trees and recursive trees, we make use of the following general limit theorem of additive parameters due to Holmgren and Janson [26].

Theorem 5.4.1. *[26] Let $F(T)$ be an additive parameter of a rooted tree T with toll function $f(T)$, i.e.*

$$F(T) = \sum_{i=1}^{d} F(T_i) + f(T),$$

where $T_1, T_2, \ldots, T_d$ are the branches of T.

1. *For binary increasing trees, assume that*

$$\sum_{k=1}^{\infty} \frac{\sqrt{Var\ f(\mathbb{T}_k)}}{k^{\frac{3}{2}}} < \infty,$$
$$\lim_{k\to\infty} \frac{Var\ f(\mathbb{T}_k)}{k} = 0,$$
$$\sum_{k=1}^{\infty} \frac{(\mathbb{E}f(\mathbb{T}_k))^2}{k^2} < \infty.$$

Then, as $n \to \infty$,

$$\frac{\mathbb{E}(F(\mathbb{T}_n))}{n} \to \mu_F := \sum_{k=1}^{\infty} \frac{2}{(k+1)(k+2)} \mathbb{E}f(\mathbb{T}_k),$$
$$\frac{Var\ (F(\mathbb{T}_n))}{n} \to \sigma_F^2 := \lim_{N\to\infty} \sum_{|T|,|T'|\le N} f(T)f(T')\sigma_{T,T'} < \infty,$$

where $\sigma_{T,T'}$ is the covariance between $F(T)$ and $F(T')$ in $\mathbb{T}_n$, and

$$\frac{F(\mathbb{T}_n) - \mathbb{E}F(\mathbb{T}_n)}{\sqrt{n}} \xrightarrow{d} \mathcal{N}(0, \sigma_F^2).$$

2. *For random recursive trees, assume that*

$$\sum_{k=1}^{\infty} \frac{\sqrt{Var\ f(\mathcal{T}_k)}}{k^{\frac{3}{2}}} < \infty,$$
$$\lim_{k\to\infty} \frac{Var\ f(\mathcal{T}_k)}{k} = 0,$$
$$\sum_{k=1}^{\infty} \frac{(\mathbb{E}f(\mathcal{T}_k))^2}{k^2} < \infty.$$

Then, as $n \to \infty$,

$$\frac{\mathbb{E}(F(\mathcal{T}_n))}{n} \to \hat{\mu}_F := \sum_{k=1}^{\infty} \frac{2}{(k+1)(k+2)} \mathbb{E}f(\mathcal{T}_k),$$
$$\frac{Var\ (F(\mathcal{T}_n))}{n} \to \hat{\sigma}_F^2 := \lim_{N\to\infty} \sum_{|T|,|T'|\le N} f(T)f(T')\sigma_{T,T'} < \infty,$$

where $\sigma_{T,T'}$ is the covariance between $F(T)$ and $F(T')$ in $\mathcal{T}_n$, and

$$\frac{F(\mathcal{T}_n) - \mathbb{E}F(\mathcal{T}_n)}{\sqrt{n}} \xrightarrow{d} \mathcal{N}(0, \hat{\sigma}_F^2).$$

Remark 5.4.2. *It is clear the additive parameter $N_\alpha(T)$ with toll function $n_\alpha(T) = N_\alpha(T) - N_\alpha(T - r)$ (see Section 2.6) of an increasing tree T with root r satisfies the assumptions in Theorem 5.4.1 since we know that $n_\alpha(T) \in \{-1, 0, 1\}$, and this immediately implies that the distribution of the multiplicity of an eigenvalue α in the spectra of recursive trees and binary increasing trees converges in the limit to a normal distribution.*

Chapter 6

The ancestral matrix of a rooted tree

In this chapter, we will be interested in the combinatorial and spectral properties of a matrix associated with a rooted tree. A rooted tree has a distinguished vertex, called the root; the vertices of a rooted tree can be arranged in levels by their distance to the root: level ℓ consists of all vertices whose distance from the root is ℓ. Thus the root is the only vertex at level 0, and all the children (if there are any) of a level-ℓ vertex are at level $\ell + 1$. A vertex without children will be called a leaf; this includes the root if it is the only vertex, but not otherwise. The set of leaves of a (rooted) tree T will be denoted by $\mathcal{L}(T)$, the number of leaves by $L(T)$.

Rooted trees occur naturally in many different areas, from data structures to phylogenetics. This work is an attempt to introduce the powerful framework of spectral graph theory to the world of rooted trees by studying what will be called the ancestral matrix of a rooted tree. In order to define it formally, we need a few ingredients. A rooted tree can be regarded as the Hasse diagram of a poset, where the root is the greatest (or least if we reverse the order) element. For any two elements v, w of this poset, there is a unique supremum $v \vee w$, the least element that is simultaneously greater than or equal to both v and w. In terms of the tree structure, this can be interpreted as the lowest element (farthest from the root) that is an ancestor of both v and w. The ancestral level of v and w is the level of $v \vee w$, i.e., the greatest distance of a common ancestor from the root. We will denote it by $\ell(v \vee w)$. It is worth pointing out a connection between the ancestral level and distances: if r denotes the root and $d(\cdot, \cdot)$ the usual graph distance, then we have

$$d(v,w) = d(v,r) + d(w,r) - 2\ell(v \vee w), \tag{6.1}$$

since the path from v to r and the path from w to r both include the path from $v \vee w$ to r, while the remaining parts form the path from v to w.

The ancestral level is a way to measure how close two vertices are. For example, if we interpret the rooted tree as a phylogenetic tree (see [35]), then it represents the point at which two species are separated. In an important data structure known as a trie (see e.g. [29, Section 6.3]), where the leaves store data according to certain keys (strings over a given alphabet), the ancestral level is the length of the longest common prefix.

To define the ancestral matrix, we focus on the leaves. Let $v_1, v_2, \dots, v_n$ be the leaves of a rooted tree T. The ancestral matrix $C(T)$ is defined by its entries c_{ij} in the following way:

$$c_{ij} = \ell(v_i \vee v_j).$$

For the example in Figure 6.1, the ancestral matrix is

$$\begin{bmatrix} 2 & 1 & 0 & 0 & 0 & 0 \\ 1 & 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 1 & 1 & 1 \\ 0 & 0 & 1 & 2 & 1 & 1 \\ 0 & 0 & 1 & 1 & 3 & 2 \\ 0 & 0 & 1 & 1 & 2 & 3 \end{bmatrix}.$$

The ancestral matrix is similar in nature to a meet matrix, see [25]. Meet matrices can be defined on arbitrary posets; their determinants are particularly well-studied. Some basic properties of the ancestral matrix are immediate: it is clearly always a symmetric matrix, and the diagonal entry is always the unique maximum in each row and column.

Another important structural property relates to the branches of a rooted tree: let T_1, T_2, ..., T_k be the branches of a rooted tree T (i.e., the connected components that remain when the root of T is removed, each endowed with its natural root). For every $j \in \{1, 2, \dots, k\}$, let E_j be a square matrix whose entries are all equal to 1, and whose size (number of rows) equals the number of leaves of T_j. Then the ancestral matrix $C(T)$ has the following block

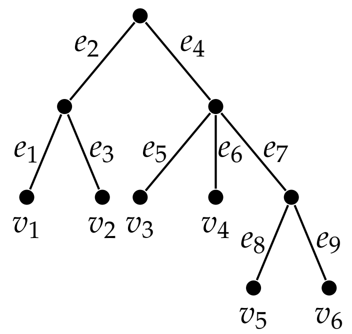


Figure 6.1: Example of a rooted tree.

diagonal form with respect to a suitable order of leaves:

$$C(T) = \begin{bmatrix} C(T_1)+E_1 & 0 & 0 & \cdots & 0 \\ 0 & C(T_2)+E_2 & 0 & \cdots & 0 \\ 0 & 0 & C(T_3)+E_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & C(T_k)+E_k \end{bmatrix}. \tag{6.2}$$

This is because the ancestral level of two leaves that lie in distinct branches is always 0, while the ancestral level of two leaves in the same branch increases by 1 in T.

The ancestral spectrum of a rooted tree T is now defined in analogy to other graph spectra (such as the adjacency spectrum or the Laplacian spectrum) as the spectrum of the ancestral matrix $C(T)$. Note that this spectrum does not depend on the order of leaves, and that all eigenvalues are necessarily real since $C(T)$ is symmetric. In the example of Figure 6.1, the eigenvalues are (in decreasing order) $4+\sqrt{5}, 3, 4-\sqrt{5}, 1, 1, 1$.

In analogy with the fact that the Laplacian and the signless Laplacian of a graph can be obtained as the product of an incidence matrix with its own transpose, a similar identity holds for the ancestral matrix. To this end, we define a path incidence matrix $I_p(T)$ of a rooted tree T. Let $P(u,v)$ be the set of edges on the path from vertex u to vertex v in a tree T. Suppose $v_1, v_2, \ldots, v_n$ and $e_1, e_2, \ldots, e_m$ are the leaves and the edges of a rooted tree T with root r. The path incidence matrix $I_p(T)$ is defined as an $n \times m$ matrix whose entries are

$$a_{ij} = \begin{cases} 1 & \text{if } e_j \in P(v_i, r), \\ 0 & \text{otherwise.} \end{cases}$$

The path incidence matrix for the rooted tree in Figure 6.1 is

$$\begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 \end{bmatrix}.$$

Note that the row sums are equal to the respective depths of the leaves and the column sums provide information on the number of leaves “below” a certain edge. It is easy to see that for a rooted tree T, we have

$$C(T) = I_p(T)I_p(T)^t.$$

An immediate consequence of this identity is the fact that the ancestral matrix is positive semidefinite (in fact positive definite, as we will see in the next section).

6.1 The eigenvalues of the ancestral matrix

This section will be devoted to the eigenvalues of the ancestral matrix of a rooted tree. The Rayleigh quotient will play an important role in this context: for a symmetric matrix A and a vector $\mathbf{x}$, it is given by

$$R(A, \mathbf{x}) = \frac{\mathbf{x}^t A\mathbf{x}}{\mathbf{x}^t\mathbf{x}}.$$

It is well known that $R(A, \mathbf{x}) = \lambda$ if $\mathbf{x}$ is an eigenvector for the eigenvalue λ, and that the greatest and least eigenvalue are given by

$$\sup_{\mathbf{x}\neq\mathbf{0}} R(A, \mathbf{x}) = \sup_{\|\mathbf{x}\|=1} R(A, \mathbf{x}) = \sup_{\|\mathbf{x}\|=1} \mathbf{x}^t A\mathbf{x} \tag{6.3}$$

and

$$\inf_{\mathbf{x}\neq\mathbf{0}} R(A, \mathbf{x}) = \inf_{\|\mathbf{x}\|=1} R(A, \mathbf{x}) = \inf_{\|\mathbf{x}\|=1} \mathbf{x}^t A\mathbf{x} \tag{6.4}$$

respectively.

We start our considerations with a lower bound on the eigenvalues. As it turns out, the eigenvalue 1 plays a specific role, which is captured in the following theorem.

Theorem 6.1.1. *If T is a rooted tree that does not only consist of the root, then all eigenvalues are greater than or equal to 1. Moreover, the multiplicity of 1 as an eigenvalue of $C(T)$ is given by*

$$\big(\text{number of leaves of } T\big) - \big(\text{number of non-root vertices of } T \text{ adjacent to a leaf}\big).$$

A basis for the eigenspace of the eigenvalue 1 is obtained in the following way: for every maximal (with respect to inclusion) r-tuple $w_1, w_2, \ldots, w_r$ of leaves that share a common parent, take all vectors with an entry 1 in the row corresponding to w_1, an entry -1 in the row corresponding to w_j for some $j \in \{2, 3, \ldots, r\}$, and otherwise zeros. Moreover, if there is at least one leaf adjacent to the root, pick one such leaf u and take the vector with an entry 1 in the row corresponding to u and otherwise zeros. The set of all these vectors is a basis for the eigenspace of 1.

Proof. We prove the statement by induction on the number of vertices. The statement is vacuously true if T has only one vertex (the root), so we consider the situation that T has one or more branches, denoted by $T_1, T_2, \ldots, T_k$. It follows from the block diagonal representation of $C(T)$ in (6.2) that the spectrum of $C(T)$ is the union of the spectra of $C(T_1) + E_1$, $C(T_2) + E_2$, etc. We consider two cases for a branch T_j:

- If T_j only consists of one vertex, then $C(T_j) + E_j$ is a 1×1-matrix whose only entry is 1. This yields an eigenvalue 1.
- If T_j has more than one vertex, then we already know that

  $$\inf_{\mathbf{x} \neq \mathbf{0}} R(C(T_j), \mathbf{x}) \geq 1$$

  by the induction hypothesis. Moreover, since E_j is positive semidefinite, we have $R(E_j, \mathbf{x}) \geq 0$ with equality if and only if $\mathbf{x}$ is orthogonal to the all-1 vector $\mathbf{1}$, or equivalently if the sum of all entries of $\mathbf{x}$ is 0. Thus

  $$\inf_{\mathbf{x} \neq \mathbf{0}} R(C(T_j) + E_j, \mathbf{x}) = \inf_{\mathbf{x} \neq \mathbf{0}} \big(R(C(T_j), \mathbf{x}) + R(E_j, \mathbf{x})\big) \geq \inf_{\mathbf{x} \neq \mathbf{0}} R(C(T_j), \mathbf{x}) \geq 1 \tag{6.5}$$

  by the induction hypothesis.

It follows that every eigenvalue is greater than or equal to 1, which proves the first assertion. Now let us look at the associated eigenvectors: for each single-vertex branch, we have a unit eigenvector whose only non-zero entry

corresponds to the single vertex of the branch. If $u_1, u_2, \ldots, u_s$ are (without loss of generality) all leaves adjacent to the root, then each of them gives rise to such a unit eigenvector, and these s eigenvectors are clearly linearly independent. However, we can replace them by a different set of vectors that spans the same space: the unit vector corresponding to u_1, and for every $j > 1$ the vector with an entry 1 corresponding to u_1, an entry -1 corresponding to u_j, and otherwise zeros. This agrees with our description of eigenvectors.
For each branch T_j that is not a single vertex, we need eigenvectors that satisfy (6.5) with equality. For this purpose, $\mathbf{x}$ needs to be an eigenvector of $C(T_j)$ with respect to the eigenvalue 1, and $\mathbf{x}$ needs to be orthogonal to the all-1 vector $\mathbf{1}$. By the induction hypothesis, we have a basis for the eigenspace of 1 as an eigenvalue of $C(T_j)$, and it is clear that those eigenvectors with an entry 1 and an entry -1 form a basis of the subspace that is orthogonal to the all-1 vector $\mathbf{1}$. Thus these remain eigenvectors for $C(T)$ (when suitably padded with zeros) and form a basis for the eigenspace of 1 as an eigenvalue of $C(T_j) + E_j$. Each maximal r-tuple of leaves with a common parent vertex thus contributes $r - 1$ to the multiplicity of 1 as an eigenvalue, unless the common parent is the root, in which case the contribution is r. The formula for the multiplicity follows immediately. ■

So we know now in particular that the eigenvalues of $C(T)$ are not only real and non-negative, but even positive, unless T only has a single vertex. Next we look at the maximum eigenvalue of $C(T)$, i.e. the spectral radius, which we denote by $\rho_C(T)$ and call the ancestral spectral radius. Making use of the block diagonal shape once again, we see that the spectral radius is the maximum of the spectral radii of the matrices $C(T_1) + E_1$, $C(T_2) + E_2$, etc. By the Perron-Frobenius Theorem, the multiplicity of $\rho_C(T)$ as an eigenvalue of $C(T_j) + E_j$ is at most 1, and if $\rho_C(T)$ is an eigenvalue of $C(T_j) + E_j$, then there exists an eigenvector with positive entries for it. Hence the multiplicity of $\rho_C(T)$ is less than or equal to the root degree/number of root branches (equality can hold, e.g. if all root branches are isomorphic). In the following, we will call any eigenvector associated with $\rho_C(T)$ that has non-negative real entries a Perron vector of T.
The following proposition is analogous to the well-known fact that the spectral radius of the adjacency matrix of a graph lies between the average and the maximum degree (see for example [37, (1.5)]).

Proposition 6.1.2. *Let the total ancestral depth of a leaf v in T be defined by*

$$\mathrm{ad}(v) = \sum_{w \in \mathcal{L}(T)} \ell(v \vee w),$$

where the sum is over all leaves w. For every rooted tree T, we have

$$\frac{1}{L(T)} \sum_{v \in \mathcal{L}(T)} \mathrm{ad}(v) \leq \rho_C(T) \leq \max_{v \in \mathcal{L}(T)} \mathrm{ad}(v).$$

Proof. Note that $\mathrm{ad}(v)$ is precisely the row sum of the row that corresponds to v. For the lower bound, we consider the Rayleigh quotient of the vector $\mathbf{1}$. Since $\mathbf{1}^t\mathbf{1} = L(T)$ and $\mathbf{1}^t C(T)\mathbf{1}$ is the sum of all entries of $C(T)$, we have

$$\rho_C(T) \geq R(C(T), \mathbf{1}) = \frac{1}{L(T)} \sum_{v \in \mathcal{L}(T)} \mathrm{ad}(v).$$

For the upper bound, consider an eigenvector $\mathbf{x}$ associated with $\rho_C(T)$, and denote the entry of $\mathbf{x}$ associated with vertex v by $x(v)$. Recall that the eigenvector can be chosen to have only non-negative entries. Let w be the vertex for which $x(w)$ attains its maximum value. The eigenvalue equation gives us

$$\rho_C(T)x(w) = \sum_v \ell(v \vee w)x(v) \leq \sum_v \ell(v \vee w)x(w) = \mathrm{ad}(w)x(w),$$

thus

$$\rho_C(T) \leq \mathrm{ad}(w),$$

from which the upper bound follows immediately. ■

By means of the identity (6.1), $\mathrm{ad}(v)$ can be rewritten in terms of distances. Specifically, we have

$$\begin{aligned} \mathrm{ad}(v) &= \frac{1}{2} \sum_{w \in \mathcal{L}(T)} (d(v,r) + d(w,r) - d(v,w)) \\ &= \frac{1}{2}\big(L(T)d(v,r) + D_T(r) - D_T(v)\big), \end{aligned}$$

where $D_T(v)$ is the sum of all distances from v to the leaves of T. Summing over all leaves v, we get

$$\sum_{v \in \mathcal{L}(T)} \mathrm{ad}(v) = \frac{1}{2}\Big(2L(T)D_T(r) - \sum_{v \in \mathcal{L}(T)} D_T(v)\Big) = L(T)D_T(r) - \mathrm{TW}(T),$$

where $\mathrm{TW}(T)$ represents the terminal Wiener index, i.e. the sum of all distances between pairs of leaves:

$$\mathrm{TW}(T) = \sum_{\{v,w\} \subseteq \mathcal{L}(T)} d(v,w).$$

Hence the lower bound in Proposition 6.1.2 becomes

$$D_T(r) - \frac{\mathrm{TW}(T)}{L(T)} \leq \rho_C(T). \tag{6.6}$$

Another simple lower bound for the spectral radius $\rho_C(T)$ is given by the height $h(T)$, i.e. the greatest distance of a leaf from the root.

Proposition 6.1.3. *For every rooted tree T, we have $\rho_C(T) \geq h(T)$.*

Proof. Let v be a leaf whose distance to the root equals $h(T)$, and take $\mathbf{x}$ to be the unit vector with one entry 1 corresponding to v and otherwise only zeros. It is easy to see that $R(C(T), \mathbf{x}) = h(T)$, so the statement follows immediately from (6.3). ∎

The inequality in Proposition 6.1.3 is actually sharp for every value of $h(T)$ and every value of $L(T)$: to see this, consider a tree consisting of the root, $n-1$ leaves attached to the root, and a path of length h attached to the root (at one of its ends).
For the star S_n (consisting only of a root and n leaves attached to it), we have $\rho_C(S_n) = 1$ for every n. Thus the trivial bound $\rho_C(T) \geq 1$ is in fact sharp for all possible sizes of T. However, the lower bound can be improved if the degrees are restricted, as is shown in the following theorem:

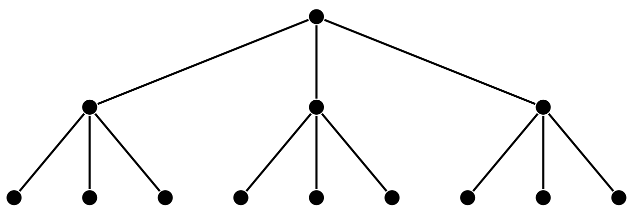


Figure 6.2: A complete ternary tree.

Theorem 6.1.4. *Let T be a rooted tree for which the outdegree (number of children) of all vertices is less than or equal to Δ. Then we have*

$$\rho_C(T) \geq \frac{L(T)-1}{\Delta - 1}.$$

Equality holds if and only if T is a complete Δ-ary tree, i.e. a rooted tree for which all leaves lie on the same level and all internal vertices have precisely Δ children; see Figure 6.2 for an example in the case $\Delta = 3$.

Proof. We make use of the lower bound of Proposition 6.1.2. It will be shown that

$$\sum_{v \in \mathcal{L}(T)} \mathrm{ad}(v) \geq \frac{L(T)(L(T)-1)}{\Delta - 1}, \tag{6.7}$$

from which the stated inequality follows. Let us use the shorthand

$$Q(T) = \sum_{v \in \mathcal{L}(T)} \mathrm{ad}(v) = \sum_{v \in \mathcal{L}(T)} \sum_{w \in \mathcal{L}(T)} \ell(v \vee w).$$

Our first goal is a recursion for this quantity in terms of the branches of T. Let these branches be denoted by $T_1, T_2, \ldots, T_k$. For two leaves v, w in distinct branches, we simply have $\ell(v \vee w) = 0$. For two leaves v, w in the same branch T_i, $\ell(v \vee w)$ increases by 1 in T compared to T_i. Thus we have

$$\begin{aligned} Q(T) &= \sum_{i=1}^{k} \Big(Q(T_i) + \sum_{v \in \mathcal{L}(T_i)} \sum_{w \in \mathcal{L}(T_i)} 1 \Big) \\ &= \sum_{i=1}^{k} \big(Q(T_i) + L(T_i)^2 \big). \end{aligned}$$

Now we prove (6.7) by induction on the number of vertices of T. If there is only one vertex, then both sides of the inequality are 0, so it holds. Otherwise, there are one or more branches $T_1, T_2, \ldots, T_k$ (where $k \leq \Delta$). The recursion for $Q(T)$, combined with the induction hypothesis, gives us

$$\begin{aligned} Q(T) &= \sum_{i=1}^{k} \big(Q(T_i) + L(T_i)^2 \big) \\ &\geq \sum_{i=1}^{k} \Big(\frac{L(T_i)(L(T_i)-1)}{\Delta - 1} + L(T_i)^2 \Big) \\ &= \frac{\Delta}{\Delta - 1} \sum_{i=1}^{k} L(T_i)^2 - \frac{1}{\Delta - 1} \sum_{i=1}^{k} L(T_i). \end{aligned}$$

We have $\sum_{i=1}^{k} L(T_i) = L(T)$, so the final term simplifies to $\frac{L(T)}{\Delta - 1}$. Moreover, the inequality between the quadratic and the arithmetic mean gives us

$$\sum_{i=1}^{k} L(T_i)^2 \geq \frac{1}{k} \Big(\sum_{i=1}^{k} L(T_i) \Big)^2 = \frac{L(T)^2}{k} \geq \frac{L(T)^2}{\Delta}.$$

Putting everything together, we obtain

$$Q(T) \geq \frac{\Delta}{\Delta - 1} \cdot \frac{L(T)^2}{\Delta} - \frac{1}{\Delta - 1} \cdot L(T) = \frac{L(T)(L(T) - 1)}{\Delta - 1},$$

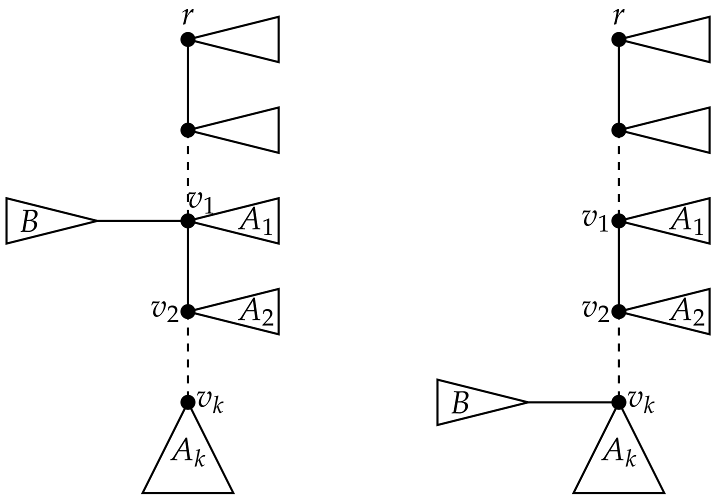
which completes the induction. Note that equality holds if and only if $k = \Delta$, $L(T_1) = L(T_2) = \cdots = L(T_k)$ and equality holds for each of the branches T_i. It is easy to deduce that equality holds if and only if T is a complete Δ-ary tree, as stated. ∎

We remark that the parameter Q is somewhat similar in its definition to the Wiener index (sum of distances between all pairs of vertices), which is known to be minimised by complete Δ-ary trees as well, see [16].

Moving our attention to upper bounds, we focus on classes of trees with fixed parameters such as outdegree sequence, number of vertices and number of leaves. The outdegree of a vertex is the number of children, and the outdegree sequence is the sequence of outdegrees of all vertices in a rooted tree. As it turns out, the maximum of the ancestral spectral radius $\rho_C(T)$ is typically attained by a so-called caterpillar tree. A rooted caterpillar T is a rooted tree with the property that removing all of its leaves yields a path with the root at one end. The resulting path is called the backbone or spine of the caterpillar T.

Before we state our results, we first introduce some useful lemmas. The main idea is to apply certain tree operations that affect the ancestral spectral radius while preserving some of the features of the tree (such as the outdegree sequence).

Firstly, we introduce an operation that moves branches away from the root along a path while preserving the number of leaves. In this way, we increase the levels of the common ancestors of some of the leaves. Formally, this operation can be described as follows: let $v_1, v_2, \ldots, v_k$ be consecutive vertices (in this order) on a path from the root to a leaf of a rooted tree T, and assume that v_k is not a leaf. Moreover, let B be a branch attached to v_1 (a subtree consisting of a child of v_1 and all its descendants). We construct a tree T' by moving B to v_k (by removing the edge between B's root and v_1 and replacing it with an edge to v_k). This is illustrated in Figure 6.3. We shall call this operation the branch shift operation. It turns out that this operation increases the ancestral spectral radius, which is captured in the following lemma.



(a) The rooted tree T. (b) The rooted tree T'.

Figure 6.3: T' is obtained from T by the branch shift operation.

Lemma 6.1.5. *Suppose that T' is obtained from a rooted tree T by the branch shift operation as described above and depicted in Figure 6.3. Assume moreover that there is a Perron vector for T with the property that the entries corresponding to leaf descendants of v_k (all leaves for which the path to the root passes through v_k) are positive. Then $\rho_C(T') > \rho_C(T)$.*

Proof. As indicated in the figure, we denote the subtree consisting of v_k and all its descendants by A_k, and we denote the subtrees consisting of $v_1, v_2, \ldots, v_{k-1}$ and all their respective descendants not lying on the path $v_1, v_2, \ldots, v_k$, the subtree A_k or the branch B by $A_1, A_2, \ldots, A_{k-1}$.
Let $\boldsymbol{f}$ be a unit Perron vector whose entries corresponding to the leaves in A_k are positive; such a vector exists by assumption. We write $f(u)$ for the entry of $\boldsymbol{f}$ corresponding to a leaf u in T. In the following, we will use ℓ_T to indicate the level of a vertex in T (to emphasize the dependence on the tree).
The main idea of the proof of this lemma is to show that the difference between the Rayleigh quotients $R(C(T'), \boldsymbol{f})$ and $R(C(T), \boldsymbol{f})$ defined on the Perron vector $\boldsymbol{f}$ of the rooted tree T is strictly positive.
Note that $\ell_{T'}(x \vee y) - \ell_T(x \vee y) = 0$ for all pairs of leaves x, y that do not belong to B. Hence we can ignore all such pairs. The same is true if x lies in B, but y does not lie in $\cup_{i=2}^{k} A_i$, or vice versa.

If x lies in B and y in A_i for some i, or vice versa, then we have

$$\ell_{T'}(x \vee y) = (i-1) + \ell_T(x \vee y).$$

Finally, if x and y are both leaves in B, then

$$\ell_{T'}(x \vee y) = (k-1) + \ell_T(x \vee y). \tag{6.8}$$

Therefore, we can deduce that the entries of the matrix $C(T')$ are greater than or equal to those of the matrix $C(T)$, and it follows that

$$\rho_C(T') \geq R(C(T'), \boldsymbol{f}) \geq R(C(T), \boldsymbol{f}) = \rho_C(T). \tag{6.9}$$

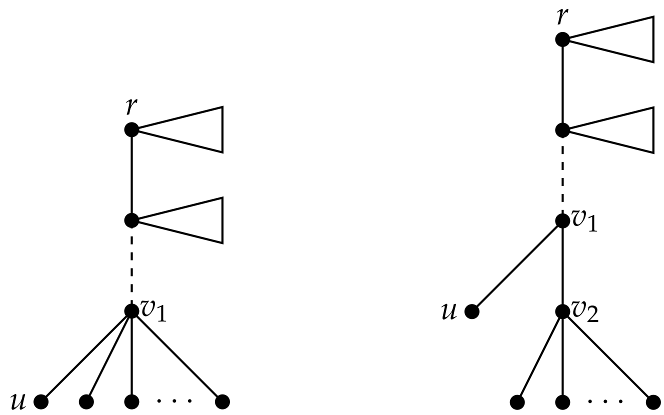
In view of (6.8), we even have

$$R(C(T'), \boldsymbol{f}) \geq R(C(T), \boldsymbol{f}) + (k-1)\Big(\sum_{u \in B} f(u)\Big)^2,$$

so equality in (6.9) can only hold if $f(u) = 0$ for all $u \in B$. Moreover, for equality to hold, $\boldsymbol{f}$ would also have to be a Perron vector of T'. But since $\boldsymbol{f}$ is non-zero on A_k by assumption, it has to be non-zero on all leaves that belong to the same root branch of T' as A_k, in particular the leaves that belong to B. Thus we must have strict inequality. In fact, this argument even shows that $f(u) = 0$ is only possible in T for leaves $u \in B$ if v_1 is the root. Hence the statement of the lemma holds. ∎

Another important tree operation that increases the ancestral spectral radius of a rooted tree is the star shift operation. This operation increases the number of internal vertices by 1, but preserves the number of leaves in the tree. Let v_1 be a vertex of a rooted tree T all of whose (at least two) children are leaves, and let u be one of these leaves. The star shift operation introduces a new vertex v_2, which becomes a child of v_1. The leaf u remains a child of v_1, while all other children of v_1 become children of v_2. The result is a tree T', see Figure 6.4 for an illustration.

Lemma 6.1.6. *Suppose that T' is obtained from a rooted tree T by the star shift operation as described above and depicted in Figure 6.4. Assume moreover that there is a Perron vector for T with the property that the entries corresponding to children of v_1 are positive. Then $\rho_C(T') > \rho_C(T)$.*



(a) The rooted tree T. (b) The rooted tree T'.

Figure 6.4: T' is obtained from T by the star shift operation.

Proof. We let $\boldsymbol{f}$ be a unit Perron vector with the property that the entries corresponding to children of v_1 are positive. Observe that

$$\ell_{T'}(x \vee y) - \ell_T(x \vee y) = 0$$

unless both x and y are children of v_2 in T'. In the latter case, we have

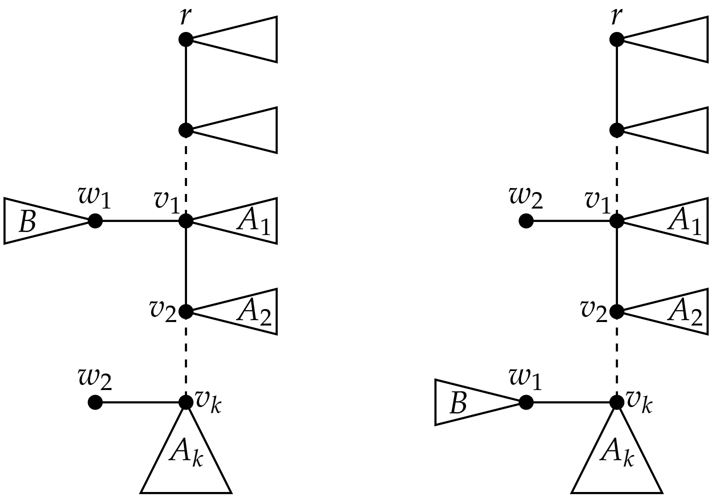
$$\ell_{T'}(x \vee y) - \ell_T(x \vee y) = 1$$

So as in the previous lemma, the entries of the matrix $C(T')$ are greater than or equal to those of the matrix $C(T)$. This together with the assumption that the entries of $\boldsymbol{f}$ corresponding to the children of v_2 are positive shows that

$$\rho_C(T') \geq R(C(T'), \boldsymbol{f}) > R(C(T), \boldsymbol{f}) = \rho_C(T).$$

■

Finally, we introduce the leaf swap operation (LSO). Similar to the branch shift operation, it moves branches away from the root. The setup is depicted in Figure 6.5. An important feature of this operation is that it does not change the outdegree sequence. As in the setup of the branch shift operation, we let $v_1, v_2, \dots, v_k$ be consecutive vertices (in this order) on a path from the root to a leaf of a tree T, and assume that v_k is not a leaf. Moreover, w_1 and w_2 are children of v_1 and v_k respectively such that w_2 is a leaf while w_1 is not. The leaf swap operation takes the subtree B induced by w_1 and all its successors and swaps it with w_2 (equivalently, the edges v_1w_1 and v_kw_2 are removed and replaced by edges v_1w_2 and v_kw_1). This is illustrated in Figure 6.5.



(a) The rooted tree T. (b) The rooted tree T'.

Figure 6.5: T' is obtained from T by the leaf swap operation.

Lemma 6.1.7. *Suppose that T' is obtained from a rooted tree T by the leaf swap operation as described above and depicted in Figure 6.5. Assume moreover that there is a Perron vector for T with the property that the entries corresponding to leaf descendants of v_k (all leaves for which the path to the root passes through v_k) are positive. Then $\rho_C(T') > \rho_C(T)$.*

Proof. As indicated in Figure 6.5, we define subtrees $A_1, A_2, \ldots, A_k$ in a similar fashion as in the proof of Lemma 6.1.5. Let $\boldsymbol{f}$ be a unit Perron vector for which the entries corresponding to w_2 and all leaves in A_k are positive; such a vector exists by assumption. We write $f(u)$ for the entry of $\boldsymbol{f}$ corresponding to a leaf u in T. For a subtree S of T, we set

$$|S|_{\boldsymbol{f}} = \sum_{x \in \mathcal{L}(S)} f(x).$$

To prove Lemma 6.1.7, we would once again like to show that the difference $R(C(T'), \boldsymbol{f}) - R(C(T), \boldsymbol{f})$ is positive. However, since this is not always the case, we will need to distinguish different cases. We have

$$\begin{aligned} R(C(T'), \boldsymbol{f}) - R(C(T), \boldsymbol{f}) = 2 &\sum_{\{x,y\} \subseteq \mathcal{L}(T)} [\ell_{T'}(x \vee y) - \ell_T(x \vee y)] f(x) f(y) \\ &+ \sum_{z \in \mathcal{L}(T)} [\ell_{T'}(z \vee z) - \ell_T(z \vee z)] f(z)^2. \end{aligned}$$

Now note that $\ell_{T'}(x \vee y) = \ell_T(x \vee y)$, unless x or y (or both) lie in $B \cup \{w_2\}$. We consider cases where the difference $\ell_{T'}(x \vee y) - \ell_T(x \vee y)$ is not equal to 0. This happens

- when $x \in B$ and $y \in A_i$, $i \in \{2, \ldots, k\}$; then we have $\ell_{T'}(x \vee y) - \ell_T(x \vee y) = i - 1$.
- when $x = w_2$ and $y \in A_i$, $i \in \{2, \ldots, k\}$; then we have $\ell_{T'}(x \vee y) - \ell_T(x \vee y) = 1 - i$.
- when $x, y \in B$; then we have $\ell_{T'}(x \vee y) - \ell_T(x \vee y) = k - 1$.
- when $x = y = w_2$; then we have $\ell_{T'}(x \vee y) - \ell_T(x \vee y) = 1 - k$.

Combining all cases, we find that

$$R(C(T'), \boldsymbol{f}) - R(C(T), \boldsymbol{f}) = 2\sum_{i=2}^{k}(i-1)L(A_i)_{\boldsymbol{f}}(|B|_{\boldsymbol{f}} - f(w_2)) + (k-1)(|B|_{\boldsymbol{f}}^2 - f(w_2)^2).$$

Suppose first that $|B|_{\boldsymbol{f}} \geq f(w_2)$. Then it follows immediately that

$$\rho_C(T') \geq R(C(T'), \boldsymbol{f}) \geq R(C(T), \boldsymbol{f}) = \rho_C(T).$$

For equality to hold, $\boldsymbol{f}$ would also have to be an eigenvector for $C(T')$ corresponding to the eigenvalue $\rho_C(T') = \rho_C(T)$. But then it follows that

$$\begin{aligned}
0 = \rho_C(T)f(w_2) - \rho_C(T')f(w_2) &= \sum_{v \in \mathcal{L}(T)} \ell_T(v \vee w_2)f(v) - \sum_{v \in \mathcal{L}(T')} \ell_{T'}(v \vee w_2)f(v) \\
&= \sum_{v \in \mathcal{L}(T)} [\ell_T(v \vee w_2) - \ell_{T'}(v \vee w_2)]f(v) \\
&= (k-1)f(w_2) + \sum_{i=2}^{k}(i-1)|A_i|_{\boldsymbol{f}} \\
&\geq (k-1)f(w_2) > 0.
\end{aligned}$$

This contradiction shows that equality cannot hold. Hence we have $\rho_C(T') > \rho_C(T)$ if $|B|_{\boldsymbol{f}} \geq f(w_2)$.

Now consider the second case that $0 < |B|_{\boldsymbol{f}} < f(w_2)$. Then we define a vector $\boldsymbol{g}$ whose entries are given by

$$g(u) = \begin{cases} |B|_{\boldsymbol{f}} & \text{if } u = w_2, \\ \frac{f(u)f(w_2)}{|B|_{\boldsymbol{f}}} & \text{if } u \in B, \\ f(u) & \text{otherwise.} \end{cases}$$

This definition implies that $|B|_{\boldsymbol{g}} = f(w_2)$ and $|B|_{\boldsymbol{f}} = g(w_2)$. Moreover, we have $\ell_{T'}(x \vee y) = \ell_T(x \vee y)$ if $x, y \notin \mathcal{L}(B) \cup \{w_2\}$, $\ell_{T'}(x \vee y) = \ell_T(w_2 \vee y)$ and $\ell_{T'}(w_2 \vee y) = \ell_T(x \vee y)$ if $x \in \mathcal{L}(B)$ and $y \notin \mathcal{L}(B) \cup \{w_2\}$, and finally $\ell_{T'}(x \vee w_2) = \ell_T(x \vee w_2) = \ell_T(v_1)$ if $x \in \mathcal{L}(B)$. This means that most terms in the difference $\boldsymbol{g}^t C(T')\boldsymbol{g} - \boldsymbol{f}^t C(T)\boldsymbol{f}$ cancel. We are only left with

$$\begin{aligned}
\boldsymbol{g}^t C(T')\boldsymbol{g} - \boldsymbol{f}^t C(T)\boldsymbol{f} &= \sum_{x\in\mathcal{L}(B)} \sum_{y\in\mathcal{L}(B)} [g(x)g(y)\ell_{T'}(x \vee y) - f(x)f(y)\ell_T(x \vee y)] \\
&\quad + g(w_2)^2\ell_{T'}(w_2) - f(w_2)^2\ell_T(w_2) \\
&= \sum_{x\in\mathcal{L}(B)} \sum_{y\in\mathcal{L}(B)} [(g(x)g(y) - f(x)f(y))\ell_T(x \vee y) + (k-1)g(x)g(y)] \\
&\quad + (g(w_2)^2 - f(w_2)^2)\ell_T(w_2) - g(w_2)^2(k-1) \\
&= \left(\frac{f(w_2)^2}{|B|_{\boldsymbol{f}}^2} - 1\right) \sum_{x\in\mathcal{L}(B)} \sum_{y\in\mathcal{L}(B)} f(x)f(y)\ell_T(x \vee y) + (k-1)|B|_{\boldsymbol{g}}^2 \\
&\quad + (g(w_2)^2 - f(w_2)^2)\ell_T(w_2) - g(w_2)^2(k-1).
\end{aligned}$$

Since $\ell_T(x \vee y) \geq \ell_T(v_1) + 1$ for all $x, y \in \mathcal{L}(B)$, it follows that

$$\begin{aligned}
\boldsymbol{g}^t C(T')\boldsymbol{g} - \boldsymbol{f}^t C(T)\boldsymbol{f} &\geq \left(\frac{f(w_2)^2}{g(w_2)^2} - 1\right) \sum_{x\in\mathcal{L}(B)} \sum_{y\in\mathcal{L}(B)} f(x)f(y)(\ell_T(v_1) + 1) + (k-1)f(w_2)^2 \\
&\quad + (g(w_2)^2 - f(w_2)^2)\ell_T(w_2) - g(w_2)^2(k-1) \\
&= \left(\frac{f(w_2)^2}{g(w_2)^2} - 1\right)|B|_{\boldsymbol{f}}^2(\ell_T(v_1) + 1) + (g(w_2)^2 - f(w_2)^2)(\ell_T(w_2) - k + 1) \\
&= \left(\frac{f(w_2)^2}{g(w_2)^2} - 1\right)g(w_2)^2(\ell_T(v_1) + 1) + (g(w_2)^2 - f(w_2)^2)(\ell_T(v_1) + 1) \\
&= 0.
\end{aligned}$$

Moreover, we have (since $\boldsymbol{f}$ was assumed to be a unit vector)

$$1 = \|\boldsymbol{f}\|^2 = f(w_2)^2 + \sum_{u\in\mathcal{L}(B)} f(u)^2 + \sum_{u\notin\mathcal{L}(B)\cup\{w_2\}} f(u)^2$$

and

$$\|\boldsymbol{g}\|^2 = |B|_{\boldsymbol{f}}^2 + \frac{f(w_2)^2}{|B|_{\boldsymbol{f}}^2}\left(\sum_{u\in\mathcal{L}(B)} f(u)^2\right) + \sum_{u\notin\mathcal{L}(B)\cup\{w_2\}} f(u)^2,$$

thus

$$\begin{aligned}\|\boldsymbol{f}\|^2 - \|\boldsymbol{g}\|^2 &= f(w_2)^2\Big(1 - \frac{\sum_{u\in\mathcal{L}(B)} f(u)^2}{|B|_{\boldsymbol{f}}^2}\Big) + \sum_{u\in\mathcal{L}(B)} f(u)^2 - |B|_{\boldsymbol{f}}^2 \\ &= f(w_2)^2\Big(\frac{|B|_{\boldsymbol{f}}^2 - \sum_{u\in\mathcal{L}(B)} f(u)^2}{|B|_{\boldsymbol{f}}^2}\Big) - \Big(|B|_{\boldsymbol{f}}^2 - \sum_{u\in\mathcal{L}(B)} f(u)^2\Big) \\ &= \Big(|B|_{\boldsymbol{f}}^2 - \sum_{u\in\mathcal{L}(B)} f(u)^2\Big)\Big(\frac{f(w_2)^2}{|B|_{\boldsymbol{f}}^2} - 1\Big).\end{aligned}$$

The second factor is strictly positive since $|B|_{\boldsymbol{f}} < f(w_2)$ by assumption. The first factor is non-negative, since we can write it as

$$|B|_{\boldsymbol{f}}^2 - \sum_{u\in\mathcal{L}(B)} f(u)^2 = \sum_{u\in\mathcal{L}(B)} \sum_{v\in\mathcal{L}(B)\setminus\{u\}} f(u)f(v).$$

Moreover, since $|B|_{\boldsymbol{f}} > 0$, we must have $f(u) > 0$ for all $u \in \mathcal{L}(B)$ (if one of them is positive, all of them are, since the leaves of B belong to the same root branch). So if B contains at least two leaves, then the first factor is also strictly positive.

Thus we conclude that $\|\boldsymbol{g}\| \leq \|\boldsymbol{f}\| = 1$, with strict inequality if B contains at least two leaves. If this is the case, we can combine it with the inequality

$$\boldsymbol{g}^t C(T')\boldsymbol{g} - \boldsymbol{f}^t C(T)\boldsymbol{f} \geq 0 \tag{6.10}$$

that was proven earlier to obtain

$$\rho_C(T') \geq R(C(T'), \boldsymbol{g}) > R(C(T), \boldsymbol{f}) = \rho_C(T). \tag{6.11}$$

If B only contains one leaf, then the assumption that B is not just a single vertex allows us to replace the inequality $\ell_T(x \vee y) \geq \ell_T(v_1) + 1$ that was used earlier by the stronger version $\ell_T(x \vee y) \geq \ell_T(v_1) + 2$, giving us strict inequality in (6.10). Once again, we have (6.11), which completes the proof in this case.

Finally, in the third case that $|B|_{\boldsymbol{f}} = 0$, we set

$$g(u) = \begin{cases} 0 & \text{if } u = w_2, \\ \frac{f(w_2)}{L(B)} & \text{if } u \in B, \\ f(u) & \text{otherwise.}\end{cases}$$

Then we can proceed in exactly the same way as in the second case. ∎

Remark 6.1.8. *In each of the three preceding lemmas, the assumption on the Perron vector is essential to ensure strict inequality. Otherwise, we only get* $\rho_C(T') \geq \rho_C(T)$ *from the three operations.*

A greedy caterpillar (see Figure 6.6) is a rooted caterpillar with the property that the outdegrees of its internal vertices increase along the backbone. Given an outdegree sequence S, we can construct a greedy caterpillar $G(S)$ by the following steps:

- Construct the backbone, which is a path whose length is the number of non-zero entries in the outdegree sequence S.
- Assign the lowest non-zero entry in S (say, s) to the root (one end of the backbone) by attaching $s - 1$ leaves to it.
- Assign, in ascending order, non-zero entries in S to the vertices on the backbone with respect to their distance from the root by attaching a suitable number of leaves.

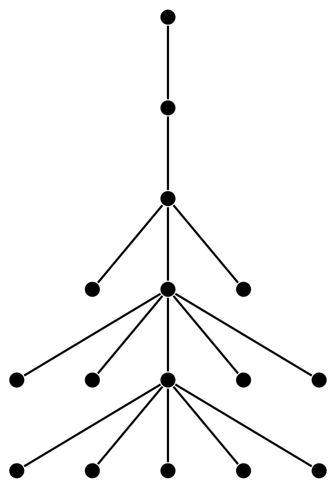


Figure 6.6: A greedy caterpillar with outdegree sequence $(5, 5, 3, 1, 1, 0, \ldots, 0)$.

Theorem 6.1.9. *Among all trees with outdegree sequence* S*, the greedy caterpillar* $G(S)$ *has the maximum ancestral spectral radius.*

Proof. To prove this theorem we show that a greedy caterpillar T' can be obtained from any rooted tree T with the same outdegree sequence by the

branch shift and the leaf swap operation. Hence by Lemma 6.1.5 and Lemma 6.1.7, we obtain the statement of the theorem.
If T is already a caterpillar, but not a greedy caterpillar, then we can easily obtain the greedy caterpillar $G(S)$ by shifting leaves along its backbone (repeatedly applying the branch shift operation) without changing the outdegree sequence. Therefore by Lemma 6.1.5, we get that $\rho_C(G(S)) > \rho_C(T)$.
Otherwise, we transform T into a caterpillar. Consider the vertex closest to the root (possibly the root itself) that has more than one non-leaf child, and call it v_1. Moreover, let $\boldsymbol{f}$ be a Perron vector associated with T. At least one of the branches rooted at the children of v_1 must contain leaves for which the corresponding entries of $\boldsymbol{f}$ are positive: if not, then the positive entries of $\boldsymbol{f}$ would have to lie in a root branch to which v_1 does not belong, which would have to be a leaf. In this case, we would have $\rho_C(T) = 1$, which is impossible.
In the aforementioned branch of v_1, we can find a vertex v_k with a leaf child w_2, and there is also a branch of v_1 (rooted at a child w_1 of v_1) that is not just a single vertex. Thus we are in the situation where the leaf swap operation applies, so we can construct a new tree T' with the same outdegree sequence such that $\rho_C(T') > \rho_C(T)$. This procedure can be repeated until we obtain a caterpillar. ∎

There are similar examples where "greedy" structures maximise the spectral radius; for instance, this is the case for the spectral radius and Laplacian spectral radius of trees [6, 39].
An immediate consequence of Theorem 6.1.9 is Theorem 6.1.10 below, which deals with trees for which the number of leaves and the number of vertices are given. A rooted broom $B_{m,n}$ is a rooted tree obtained by attaching n leaves to one end of a path of length m, the other end being the root. Thus a rooted broom $B_{m,n}$ has n leaves and $m + n + 1$ vertices.

Theorem 6.1.10. *The rooted broom $B_{N-n-1,n}$ maximises the ancestral spectral radius among all rooted trees with N vertices and n leaves. We have*

$$\rho_C(B_{N-n-1,n}) = n(N - n - 1) + 1.$$

Proof. By the previous theorem, it is clear that the tree with greatest ancestral spectral radius among all such rooted trees has to be a greedy caterpillar. Applying the branch shift operation repeatedly to the leaves of such a

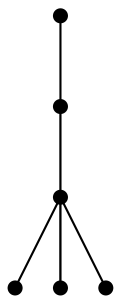


Figure 6.7: The rooted broom $B(2,3)$.

greedy caterpillar to transfer all leaves to the lowest internal vertex, we obtain a rooted broom at the end, and the ancestral spectral radius increases with each step by Lemma 6.1.5.

To complete the proof, we only need to determine the value of $\rho_C(B_{N-n-1,n})$. Here, we note that the entries of $C(B_{N-n-1,n})$ are all equal to $N-n-1$, except for those on the diagonal, which are equal to $N-n$. We see that 1 is an eigenvalue of multiplicity $n-1$, the remaining eigenvalue being $n(N-n)-(n-1) = n(N-n-1)+1$. ∎

Next, we consider another type of restriction on the degrees. We first observe that $\rho_C(T)$ is unbounded even if the number of leaves $L(T)$ is fixed: for instance, one can consider the rooted brooms from the previous theorem. This changes, however, if we forbid vertices of outdegree 1. A tree with this property is called homeomorphically irreducible, series-reduced or topological. It turns out that the binary caterpillar tree is extremal in this case. The binary caterpillar C_n (see Figure 6.8) is the rooted tree in which all $n-1$ internal vertices form a path with the root at one of its ends, and each of them has precisely two children. Note that there are precisely n leaves. We have the following theorem.

Theorem 6.1.11. *For every rooted tree T with n leaves and no vertices whose outdegree is* 1, *we have*

$$\rho_C(T) \leq \rho_C(C_n).$$

Proof. Again, Theorem 6.1.9 immediately shows that the maximum has to be attained by a greedy caterpillar. If this caterpillar is not the binary caterpillar C_n, then the internal vertex whose distance from the root is greatest must have at least three children. But then we can apply the star shift opera-

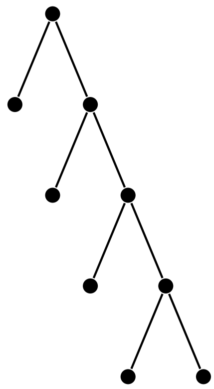


Figure 6.8: The binary caterpillar C_5.

tion to obtain a new tree that still does not contain any vertices of outdegree 1 whose ancestral spectral radius is greater by Lemma 6.1.6.
This contradiction shows that C_n must indeed attain the maximum, which is exactly the statement of the theorem. ∎

Theorem 6.1.11 raises the question for the value of $\rho_C(C_n)$. While there is no exact formula, we will be able to provide an implicit equation and an asymptotic formula in the following. To this end, we first determine a recursion for the characteristic polynomial of $C(C_n)$: set

$$P_n(x) = \det(xI - C(C_n)). \tag{6.12}$$

Proposition 6.1.12. *Let $P_n(x)$ be the characteristic polynomial of the ancestral matrix of the binary caterpillar C_n, as defined in* (6.12)*. The following recursion holds:*

$$P_n(x) = (2x-3)P_{n-1}(x) - (x-1)^2 P_{n-2}(x),$$

with initial values $P_1(x) = x$ and $P_2(x) = (x-1)^2$.

Proof. The initial values are easily determined from the matrices

$$C(C_1) = \begin{bmatrix} 0 \end{bmatrix} \qquad \text{and} \qquad C(C_2) = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},$$

so we focus on the recursion. The ancestral matrix of the caterpillar C_n has the form

$$C(C_n) = \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 2 & 1 & 1 & \cdots & 1 & 1 \\ 0 & 1 & 3 & 2 & \cdots & 2 & 2 \\ 0 & 1 & 2 & 4 & \cdots & 3 & 3 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 1 & 2 & 3 & \cdots & n-1 & n-2 \\ 0 & 1 & 2 & 3 & \cdots & n-2 & n-1 \end{bmatrix}.$$

We will also need the following auxiliary matrix, which only differs in the last entry:

$$H_n = \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 2 & 1 & 1 & \cdots & 1 & 1 \\ 0 & 1 & 3 & 2 & \cdots & 2 & 2 \\ 0 & 1 & 2 & 4 & \cdots & 3 & 3 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 1 & 2 & 3 & \cdots & n-1 & n-2 \\ 0 & 1 & 2 & 3 & \cdots & n-2 & n \end{bmatrix}.$$

Note that the $(n-1) \times (n-1)$ submatrix obtained by removing the last row and column is the same for $C(C_n)$ and H_n, namely H_{n-1}. Using the linearity of the determinant with respect to the last row, we get

$$P_n(x) = \det(xI - C(C_n)) = \begin{vmatrix} x-1 & 0 & \cdots & 0 & 0 \\ 0 & x-2 & \cdots & -1 & -1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & -1 & \cdots & x-n+1 & 2-n \\ 0 & -1 & \cdots & 2-n & x-n+1 \end{vmatrix}$$

$$= \begin{vmatrix} x-1 & 0 & \cdots & 0 & 0 \\ 0 & x-2 & \cdots & -1 & -1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & -1 & \cdots & x-n+1 & 2-n \\ 0 & -1 & \cdots & 2-n & x-n \end{vmatrix} + \begin{vmatrix} x-1 & 0 & \cdots & 0 & 0 \\ 0 & x-2 & \cdots & -1 & -1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & -1 & \cdots & x-n+1 & 2-n \\ 0 & 0 & \cdots & 0 & 1 \end{vmatrix},$$

so

$$P_n(x) = \det(xI - C(C_n)) = \det(xI - H_n) + \det(xI - H_{n-1}). \tag{6.13}$$

On the other hand, subtracting the second-to-last row from the last, then the second-to-last column from the last, we find that

$$\begin{aligned}
P_n(x) &= \det(xI - C(C_n)) \\
&= \begin{vmatrix}
x-1 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & x-2 & -1 & -1 & \cdots & -1 & -1 \\
0 & -1 & x-3 & -2 & \cdots & -2 & -2 \\
0 & -1 & -2 & x-4 & \cdots & -3 & -3 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & -1 & -2 & -3 & \cdots & x-n+1 & 2-n \\
0 & -1 & -2 & -3 & \cdots & 2-n & x-n+1
\end{vmatrix} \\
&= \begin{vmatrix}
x-1 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & x-2 & -1 & -1 & \cdots & -1 & -1 \\
0 & -1 & x-3 & -2 & \cdots & -2 & -2 \\
0 & -1 & -2 & x-4 & \cdots & -3 & -3 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & -1 & -2 & -3 & \cdots & x-n+1 & 2-n \\
0 & 0 & 0 & 0 & \cdots & 1-x & x-1
\end{vmatrix} \\
&= \begin{vmatrix}
x-1 & 0 & 0 & 0 & \cdots & 0 & 0 \\
0 & x-2 & -1 & -1 & \cdots & -1 & 0 \\
0 & -1 & x-3 & -2 & \cdots & -2 & 0 \\
0 & -1 & -2 & x-4 & \cdots & -3 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & -1 & -2 & -3 & \cdots & x-n+1 & 1-x \\
0 & 0 & 0 & 0 & \cdots & 1-x & 2x-2
\end{vmatrix}.
\end{aligned}$$

Now use row expansion with respect to the last row, followed by column expansion with respect to the last column. This yields

$$P_n(x) = (2x-2)\det(xI - H_{n-1}) - (1-x)^2 \det(xI - H_{n-2}).$$

Combining this with (6.13), we find

$$\det(xI - H_n) = (2x-3)\det(xI - H_{n-1}) - (1-x)^2 \det(xI - H_{n-2}).$$

Invoking (6.13) once again, we end up with

$$\begin{aligned}P_n(x) &= \det(xI - H_n) + \det(xI - H_{n-1})\\ &= (2x-3)\big(\det(xI - H_{n-1}) + \det(xI - H_{n-2})\big)\\ &\quad - (1-x)^2\big(\det(xI - H_{n-2}) + \det(xI - H_{n-3})\big)\\ &= (2x-3)P_{n-1}(x) - (x-1)^2 P_{n-2}(x).\end{aligned}$$

This completes the proof. ∎

The polynomial $P_n(x)$ can be expressed in terms of Chebyshev polynomials. Chebyshev polynomials also occur, for example, in the characteristic polynomials (with respect to the adjacency matrix) of the path and the cycle, see e.g. [1, Section 3.1]. Recall that the Chebyshev polynomials $T_n(x)$ and $U_n(x)$ are given by the recursions

$$T_0(x) = 1,\ T_1(x) = x,\ T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$$

and

$$U_0(x) = 1,\ U_1(x) = 2x,\ U_n(x) = 2xU_{n-1}(x) - U_{n-2}(x).$$

If we substitute $P_n(x) = (x-1)^n Q_n(x)$, then the recursion of Proposition 6.1.12 becomes

$$Q_n(x) = \frac{2x-3}{x-1}Q_{n-1}(x) - Q_{n-2}(x),$$

with the initial values $Q_1(x) = \frac{x}{x-1}$ and $Q_2(x) = 1$. We observe that $Q_n(x)$ satisfies the same linear recursion as $T_n(\frac{2x-3}{2x-2})$ and $U_n(\frac{2x-3}{2x-2})$ or any linear combination of these two. It is easy to verify that

$$\frac{2x}{2x-3}T_{n-2}\Big(\frac{2x-3}{2x-2}\Big) - \frac{3}{2x-3}U_{n-2}\Big(\frac{2x-3}{2x-2}\Big)$$

has the same values for $n = 2$ and $n = 3$ as Q_n, and since they satisfy the same second-order linear recursion, we must have

$$Q_n(x) = \frac{2x}{2x-3}T_{n-2}\Big(\frac{2x-3}{2x-2}\Big) - \frac{3}{2x-3}U_{n-2}\Big(\frac{2x-3}{2x-2}\Big)$$

for all $n \geq 2$, thus

$$P_n(x) = (x-1)^n\Big(\frac{2x}{2x-3}T_{n-2}\Big(\frac{2x-3}{2x-2}\Big) - \frac{3}{2x-3}U_{n-2}\Big(\frac{2x-3}{2x-2}\Big)\Big). \tag{6.14}$$

The Chebyshev polynomials are well known to be connected to trigonometric functions by the identities

$$T_n(\cos t) = \cos(nt) \qquad \text{and} \qquad U_n(\cos t) = \frac{\sin((n+1)t)}{\sin t}.$$

This motivates the substitution $\frac{2x-3}{2x-2} = \cos t$ (equivalently, $x = 1 + \frac{1}{4\sin^2(t/2)}$) in (6.14), which gives us

$$P_n(x) = (2\sin(t/2))^{-2n}\Big(\Big(\frac{3}{\cos t} - 2\Big)\cos((n-2)t) - \Big(\frac{3}{\cos t} - 3\Big)\frac{\sin((n-1)t)}{\sin t}\Big).$$

Now use the addition theorem for the sine function to rewrite $\sin((n-1)t)$ as $\sin((n-2)t)\cos t + \cos((n-2)t)\sin t$, which results in the following simplified expression:

$$P_n(x) = \frac{1}{(2\sin(t/2))^{2n}\sin t}\Big(\sin t\cos((n-2)t) - 3(1-\cos t)\sin((n-2)t)\Big).$$

Thus the characteristic equation $P_n(x) = 0$ reduces to

$$\sin t\cos((n-2)t) = 3(1-\cos t)\sin((n-2)t)$$

or

$$\cot((n-2)t) = \frac{3(1-\cos t)}{\sin t} = 3\tan(t/2). \tag{6.15}$$

The following asymptotic formula is now a fairly straightforward consequence:

Theorem 6.1.13. *The spectral radius of the ancestral matrix of the caterpillar C_n satisfies the asymptotic formula*

$$\rho_C(C_n) = \frac{4n^2}{\pi^2} - \frac{4n}{\pi^2} + O(1)$$

as $n \to \infty$.

Proof. Recall that $x = 1 + \frac{1}{4\sin^2 t/2}$ in (6.15). The greatest eigenvalue thus corresponds to the smallest positive value of t (which we will denote by t_0) that satisfies

$$\cot((n-2)t) = 3\tan(t/2). \tag{6.16}$$

For large n, we know that the right side is positive and increasing for $t \in (0, \frac{\pi}{2(n-2)})$, while the left side is decreasing and covers the entire range from

0 to ∞. Thus there must be a (unique) solution in that interval by the intermediate value theorem. Since we are looking for the smallest positive t that satisfies (6.16), we can conclude that $t_0 < \frac{\pi}{2(n-2)}$, thus $t_0 \to 0$ as $n \to \infty$. So $\cot((n-2)t_0)$ must be close to 0, and since $\frac{\pi}{2}$ is the smallest positive zero of the cotangent, we infer that $t_0 \sim \frac{\pi}{2n}$. Thus

$$\cot((n-2)t_0) = 3\tan(t_0/2) \sim \frac{3\pi}{4n},$$

and the Taylor approximation of the cotangent yields a second-order approximation for t_0:

$$\cot((n-2)t_0) \sim \frac{\pi}{2} - (n-2)t_0,$$

which results in

$$t_0 - \frac{\pi}{2n} \sim -\frac{1}{n}\Big(\cot((n-2)t_0) - 2t_0\Big) = -\frac{1}{n}\Big(3\tan(t_0/2) - 2t_0\Big) \sim \frac{t_0}{2n} \sim \frac{\pi}{4n^2}.$$

Continuing in this way, one could even determine further terms of an asymptotic expansion. Since our initial substitution was $x = 1 + \frac{1}{4\sin^2 t/2}$, we have to plug the formula

$$t_0 = \frac{\pi}{2n} + \frac{\pi}{4n^2} + O(n^{-3})$$

in for t, which gives us

$$\rho(C_n) = 1 + \frac{1}{4\sin^2 t_0/2} = \frac{4n^2}{\pi^2} - \frac{4n}{\pi^2} + O(1).$$

■

6.2 Determinants and the characteristic polynomial

In this section, we take a closer look at the characteristic polynomial

$$\Gamma_T(x) = \det(xI - C(T)) = \sum_{k=0}^{n} (-1)^k \gamma_k(T) x^{n-k}.$$

Specifically, we will determine a combinatorial interpretation for the coefficients $\gamma_k(T)$ of this polynomial, similar to the classical combinatorial formulas due to Sachs [34] and Kelmans [28] for the coefficients of the characteristic polynomials of the adjacency matrix and the Laplacian matrix, respectively (see e.g. [11, Sections 1.4 and 1.5]). Moreover, using a recursive

approach similar to the proof of Proposition 6.1.12, we find that specific values of the characteristic polynomial are independent of the precise structure of the tree when d-ary trees are considered, see Theorem 6.2.3.
A very basic observation can be made about the coefficient $\gamma_1(T)$, which is equal to the trace of $C(T)$ and thus also the sum of the eigenvalues.

Proposition 6.2.1. *Let T be a rooted tree with root r and n leaves, and let $\alpha_1, \alpha_2, \ldots, \alpha_n$ be the eigenvalues of its ancestral matrix $C(T)$. We have*

$$\gamma_1(T) = \sum_{k=1}^{n} \alpha_k = \operatorname{tr}(C(T)) = D_T(r),$$

where $D_T(r)$ denotes the sum of the distances of all leaves to the root.

Proof. The identity of the first three expressions is basic linear algebra. To see that $\operatorname{tr}(C(T))$ equals $D_T(r)$, simply note that the diagonal entry in $C(T)$ corresponding to a leaf equals the level (distance to the root) of that leaf. ∎

The general interpretation of the coefficients $\gamma_k(T)$ is somewhat more involved. We need to start with a few definitions. An upward path from a leaf is a path (potentially trivial, i.e., only consisting of the leaf itself, without any edges) starting at a leaf and only moving towards the root. It is easy to see that a vertex at level ℓ has $\ell + 1$ upward paths emanating from it, including the trivial path. This will be important later. We will be specifically interested in collections of upward paths in a rooted tree, one starting from each of the leaves, that are edge-disjoint (not necessarily vertex-disjoint). See Figure 6.9 for an example of an edge-disjoint collection in the tree of Figure 6.1. These edge-disjoint collections are counted by the coefficients of the characteristic polynomial of $C(T)$. The following result and its proof are reminiscent of the well-known Lindström-Gessel-Viennot Lemma ([19], see also for example [1, Section 5.4]).

Theorem 6.2.2. *Let*

$$\Gamma_T(x) = \det(xI - C(T)) = \sum_{k=0}^{n} (-1)^k \gamma_k(T) x^{n-k}$$

be the characteristic polynomial of the ancestral matrix $C(T)$ of a rooted tree T. The coefficient $\gamma_k(T)$ is the number of edge-disjoint collections of upward paths where exactly k of the paths are non-trivial. Consequently,

$$\det(I + C(T)) = (-1)^n \Gamma_T(-1) = \sum_{k=0}^{n} \gamma_k(T)$$

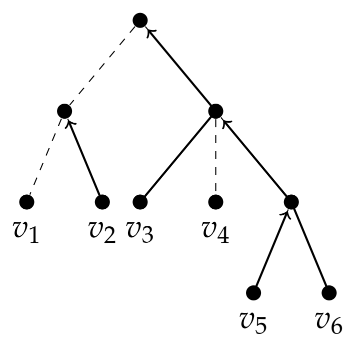


Figure 6.9: An edge-disjoint collection (the paths emanating from v_1 and v_4 are trivial).

is the total number of edge-disjoint collections of upward paths.

Proof. It is slightly more convenient for the proof to replace x by $-x$ and consider

$$\det(xI + C(T)) = (-1)^n \Gamma_T(-x) = \sum_{k=0}^{n} \gamma_k(T) x^{n-k}.$$

Let m_{ij} be the entry in the i-th row, j-th column of $xI + C(T)$. By definition of $C(T)$, we have

$$m_{ij} = \begin{cases} x + \ell(v_i) & i = j, \\ \ell(v_i \vee v_j) & i \neq j. \end{cases}$$

We apply the Leibniz formula for the determinant to obtain

$$\det(xI + C(T)) = \sum_{\sigma \in S_n} \operatorname{sgn} \sigma \prod_{i=1}^{n} m_{i,\sigma(i)}. \tag{6.17}$$

We say that a collection $\mathcal{P}$ of upward paths is compatible with a permutation σ if the following holds for all i:

- the upward path P_i starting at v_i is trivial, and $\sigma(i) = i$, or
- both ends of the last edge of P_i are ancestors of $v_{\sigma(i)}$ (possibly, one of them is v_i itself if $\sigma(i) = i$).

Note that $\ell(v_i \vee v_{\sigma(i)})$ is the number of possibilities for P_i satisfying this property, except when $i = \sigma(i)$. In the latter case, the number of possibilities is $\ell(v_i) + 1$, since the trivial path is included as well. So writing $e(\mathcal{P})$ for the number of trivial paths occurring in a collection $\mathcal{P}$, we get

$$\prod_{i=1}^{n} m_{i,\sigma(i)} = \sum_{\substack{\mathcal{P} \\ \mathcal{P},\sigma \text{ compatible}}} x^{e(\mathcal{P})}.$$

We plug this into (6.17) and interchange the order of summation:

$$\det(xI + C(T)) = \sum_{\mathcal{P}} x^{e(\mathcal{P})} \sum_{\substack{\sigma \\ \mathcal{P},\sigma \text{ compatible}}} \operatorname{sgn} \sigma. \tag{6.18}$$

Suppose first that $\mathcal{P}$ is not an edge-disjoint collection (thus an "intersecting" collection). We construct another collection $\mathcal{P}^*$ in the following way: consider the (lexicographically) smallest pair of indices i, j such that the paths P_i and P_j emanating respectively from v_i and v_j have a common edge. Now $\mathcal{P}^*$ is obtained by interchanging the parts of P_i and P_j starting from the lowest common edge (going up). It is clear that this defines an involution on the set of intersecting collections of upward paths. Importantly, if $\mathcal{P}$ is compatible with σ, then $\mathcal{P}^*$ is compatible with a permutation σ^* that differs from σ only by a transposition of i and j. Since σ and σ^* have opposite signs, it follows that

$$\sum_{\substack{\sigma \\ \mathcal{P},\sigma \text{ compatible}}} \operatorname{sgn} \sigma = - \sum_{\substack{\sigma \\ \mathcal{P}^*,\sigma \text{ compatible}}} \operatorname{sgn} \sigma,$$

which means that all intersecting collections $\mathcal{P}$ cancel pairwise in (6.18) (if $\mathcal{P} = \mathcal{P}^*$, then the sum over σ is 0). Thus we are left to consider edge-disjoint collections.

Now we claim that the only permutation that is compatible with an edge-disjoint collection is the identity, from which the desired formula follows immediately. We prove this claim by induction on the number of leaves. If there is only a single leaf, then the identity is the only permutation, so the claim is trivial. Otherwise, let $\mathcal{P}$ be an edge-disjoint collection of upward paths, and consider an internal vertex w with more than one child whose level is maximal among all such vertices. Let $v_{i_1}, v_{i_2}, \ldots, v_{i_r}$ be the leaves of which w is an ancestor. By the choice of w, $r \geq 2$, and the paths from w to these leaves are pairwise edge-disjoint. Since $\mathcal{P}$ is an edge-disjoint collection, there must be at least one leaf v_{i_s} ($s \in \{1, 2, \ldots, r\}$) such that the upward path starting from v_{i_s} does not go beyond w. Thus for σ to be compatible with $\mathcal{P}$, we need to have $\sigma(i_s) = i_s$. Now remove the path between v_{i_s} and w from the tree, and invoke the induction hypothesis on the remaining tree (and the remaining collection of upward paths, which is clearly still edge-disjoint). This completes the induction and thus the proof. ∎

A d-ary tree is a rooted tree for which each internal vertex has precisely d children. For these trees, we find that the characteristic polynomial, evaluated at one specific point, only depends on the number of leaves, but not the tree itself. This is particularly interesting for binary trees ($d = 2$), where this value yields the number of edge-disjoint collections of upward paths. A comparable result is the fact that the determinant of the distance matrix of trees only depends on the number of vertices, but not the tree structure (a theorem due to Graham and Pollak [21]; see also [13, 20]).

Theorem 6.2.3. *Let T be a d-ary tree with n leaves. We have*

$$\det\Big(\frac{1}{d-1}I + C(T)\Big) = (-1)^n \Gamma_T\Big(-\frac{1}{d-1}\Big) = (d-1)^{-n} d^{d(n-1)/(d-1)}.$$

Equivalently, if $\operatorname{int}(T)$ *is the number of internal vertices,*

$$\det\big(I + (d-1)C(T)\big) = d^{d\operatorname{int}(T)}.$$

In particular, a binary tree with n leaves has 4^{n-1} edge-disjoint collections of upward paths, which is independent of the precise shape of the tree.

Proof. We prove the statement by induction on the number of internal vertices: it is well known that a d-ary tree with n leaves has $\frac{n-1}{d-1}$ internal vertices. If the tree only consists of a single leaf, so that $L(T) = n = 1$ and there are no internal vertices, the formula reduces to $\frac{1}{d-1} = \frac{1}{d-1}$ and is thus readily seen to hold.

For the induction step, consider an internal vertex v whose level is maximal. All its children are leaves, and without loss of generality we can assume that these children correspond to the last d rows of $C(T)$. Thus the matrix $C(T) + \frac{1}{d-1}I$ has the form

$$C(T) + \frac{1}{d-1}I = \begin{bmatrix} \mathbf{B} & \mathbf{a}^t & \mathbf{a}^t & \cdots & \mathbf{a}^t \\ \mathbf{a} & k+\frac{d}{d-1} & k & \cdots & k \\ \mathbf{a} & k & k+\frac{d}{d-1} & \cdots & k \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{a} & k & k & \cdots & k+\frac{d}{d-1} \end{bmatrix},$$

where $\mathbf{B}$ is a matrix, $\mathbf{a}$ a row vector, and k is the level of vertex v. If the d leaves are removed, so that v becomes a leaf, the resulting tree T' is again a d-ary tree with $L(T') = L(T) - (d-1)$ (and $\mathrm{int}(T') = \mathrm{int}(T) - 1$), and we have

$$\frac{1}{d-1} I + C(T') = \begin{bmatrix} \mathbf{B} & \mathbf{a}^t \\ \mathbf{a} & k + \frac{1}{d-1} \end{bmatrix}.$$

We shall prove that

$$\det\left(\frac{1}{d-1} I + C(T)\right) = \det\left(\frac{1}{d-1} I + C(T')\right) \cdot \frac{d^d}{(d-1)^{d-1}},$$

so that the desired formula follows directly from the induction hypothesis. To this end, we subtract the first of the final d rows of $\frac{1}{d-1} I + C(T)$ from the other $d-1$ rows, and then the second of the last d columns from the final

$d-2$ columns to obtain

$$\det\left(\frac{1}{d-1}I+C(T)\right)=\begin{vmatrix} \mathbf{B} & \mathbf{a}^t & \mathbf{a}^t & \mathbf{a}^t & \cdots & \mathbf{a}^t \\ \\ \mathbf{a} & k+\frac{d}{d-1} & k & k & \cdots & k \\ \mathbf{a} & k & k+\frac{d}{d-1} & k & \cdots & k \\ \mathbf{a} & k & k & k+\frac{d}{d-1} & \cdots & k \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{a} & k & k & k & \cdots & k+\frac{d}{d-1} \end{vmatrix}$$

$$=\begin{vmatrix} \mathbf{B} & \mathbf{a}^t & \mathbf{a}^t & \mathbf{a}^t & \cdots & \mathbf{a}^t \\ \\ \mathbf{a} & k+\frac{d}{d-1} & k & k & \cdots & k \\ \mathbf{0} & -\frac{d}{d-1} & \frac{d}{d-1} & 0 & \cdots & 0 \\ \mathbf{0} & -\frac{d}{d-1} & 0 & \frac{d}{d-1} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & -\frac{d}{d-1} & 0 & 0 & \cdots & \frac{d}{d-1} \end{vmatrix}$$

$$=\begin{vmatrix} \mathbf{B} & \mathbf{a}^t & \mathbf{a}^t & \mathbf{0}^t & \cdots & \mathbf{0}^t \\ \\ \mathbf{a} & k+\frac{d}{d-1} & k & 0 & \cdots & 0 \\ \mathbf{0} & -\frac{d}{d-1} & \frac{d}{d-1} & -\frac{d}{d-1} & \cdots & -\frac{d}{d-1} \\ \mathbf{0} & -\frac{d}{d-1} & 0 & \frac{d}{d-1} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & -\frac{d}{d-1} & 0 & 0 & \cdots & \frac{d}{d-1} \end{vmatrix}.$$

Now add each of the last $d-2$ rows to the $(d-1)$-th row from the bottom:

$$\det\left(\frac{1}{d-1}I+C(T)\right)=\begin{vmatrix} \mathbf{B} & \mathbf{a}^t & \mathbf{a}^t & \mathbf{0}^t & \cdots & \mathbf{0}^t \\ \\ \mathbf{a} & k+\frac{d}{d-1} & k & 0 & \cdots & 0 \\ \mathbf{0} & -d & \frac{d}{d-1} & 0 & \cdots & 0 \\ \mathbf{0} & -\frac{d}{d-1} & 0 & \frac{d}{d-1} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & -\frac{d}{d-1} & 0 & 0 & \cdots & \frac{d}{d-1} \end{vmatrix}.$$

Next, expand the determinant with respect to the last $d-2$ columns, one by one:

$$\det\left(\frac{1}{d-1}I + C(T)\right) = \left(\frac{d}{d-1}\right)^{d-2} \begin{vmatrix} \mathbf{B} & \mathbf{a}^t & \mathbf{a}^t \\ \mathbf{a} & k+\frac{d}{d-1} & k \\ \mathbf{0} & -d & \frac{d}{d-1} \end{vmatrix}.$$

Finally, subtract the second to last column from the last in the remaining matrix, then add $\frac{d-1}{d}$ times the last column back to the previous column:

$$\begin{aligned} \det\left(\frac{1}{d-1}I + C(T)\right) &= \left(\frac{d}{d-1}\right)^{d-2} \begin{vmatrix} \mathbf{B} & \mathbf{a}^t & \mathbf{0}^t \\ \mathbf{a} & k+\frac{d}{d-1} & -\frac{d}{d-1} \\ \mathbf{0} & -d & \frac{d^2}{d-1} \end{vmatrix} \\ &= \left(\frac{d}{d-1}\right)^{d-2} \begin{vmatrix} \mathbf{B} & \mathbf{a}^t & \mathbf{0}^t \\ \mathbf{a} & k+\frac{1}{d-1} & -\frac{d}{d-1} \\ \mathbf{0} & 0 & \frac{d^2}{d-1} \end{vmatrix} \\ &= \frac{d^d}{(d-1)^{d-1}} \begin{vmatrix} \mathbf{B} & \mathbf{a}^t \\ \mathbf{a} & k+\frac{1}{d-1} \end{vmatrix} \\ &= \det\left(\frac{1}{d-1}I + C(T')\right), \end{aligned}$$

which completes the induction. To transform

$$\det\left(\frac{1}{d-1}I + C(T)\right) = (d-1)^{-n} d^{d(n-1)/(d-1)}$$

into

$$\det\left(I + (d-1)C(T)\right) = d^{d\,\mathrm{int}(T)},$$

one simply needs to recall that $\mathrm{int}(T) = \frac{n-1}{d-1}$. The special case $d = 2$ yields the number of edge-disjoint collections of upward paths by Theorem 6.2.2.

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