DIAGRAMMATIC APPROACH TO LEAF-TO-LEAF DISTANCES IN CATALAN TREES

**A. M. GOLDSBOROUGH^{1,2}, J. M. FELLOWS², S. A. RAUTU^{2,3},
M. BATES², G. ROWLANDS² and R. A. RÖMER²**

¹Max Planck Institute for Quantum Optics

Hans-Kopfermannstr. 1

D-85748 Garching

Germany

e-mail: Andrew@Goldsborough.org.uk

²Department of Physics and Centre for Scientific Computing

University of Warwick

Coventry, CV4 7AL

UK

e-mail: R.Roemer@warwick.ac.uk

³Simons Centre for the Study of Living Machines

National Centre for Biological Sciences (TIFR)

Bellary Road, Bangalore 560065

India

e-mail: stefanar@ncbs.res.in

2010 Mathematics Subject Classification: 05C30, 05C05, 37E25.

Keywords and phrases: Catalan trees, path lengths, diagrammatic representation.

Received April 13, 2018; Revised June 2, 2018

© 2019 Scientific Advances Publishers

This work is licensed under the Creative Commons Attribution International License
(CC BY 3.0).

http://creativecommons.org/licenses/by/3.0/deed.en_US

Abstract

Tree tensor networks are extensively used for both computational and analytic study of strongly correlated quantum matter, in which their path lengths are related to correlation functions. In this context, we study the properties of leaf-to-leaf distances on *ordered* Catalan tree graphs by using a diagrammatic method. This allows us to obtain an explicit analytic formula for the generating function of the leaf-to-leaf path lengths. By using this function, the statistical moments of such path lengths can be computed exactly. Here, we show how to construct the average distances as a function of separation of the leaves from the generating function, and study their asymptotic properties. Moreover, we find that these are equivalent to the average length of paths starting from the root node, as expected by the rerooting invariance of a tree at a random vertex.

1. Introduction

The aim of our work is to give an analytic expression for the average path length between leaves in full binary trees. Similar such tree structures have been used as an analogue for connections in the Hilbert space of wave-functions in strongly disordered Heisenberg chains [1, 2], where the path lengths are believed to be related to correlation functions [3]. More generally, it has been recently argued that certain RG approaches to the Hilbert space of critical many-body interacting system in d dimensions share many of their geometric properties with $d + 1$ dimensional AdS [4, 5]. This connection is a manifestation of the so-called AdS/CFT correspondence [6] and its possible applications in condensed matter physics [7]. In these quantum systems, the leaves are ordered according to their physical position, for example, the location of magnetic ions in a quantum wire. This ordering imposes a new restriction on the tree itself and the lengths which become important are leaf-to-leaf path lengths across the *ordered* tree. Such an ordering is usually not necessary when using traditional measures of path lengths in graph theory and computer science approaches concerned with, e.g., search trees [8].

The construction of this tree of connections in Hilbert space is based on details of so-called tensor network methods [9, 10], most famous of which is the variational matrix-product state (MPS) method that underlies modern density matrix renormalisation group (DMRG) algorithms [11, 12, 13]. These provide elegant and powerful tools for the simulation of quantum many-body systems in low dimensions. The MPS can be visualised as a one dimensional chain of tensors, one for each site. There are generalisations to higher dimensions such as the projected entangled pair state (PEPS) that takes the form of a two (or higher) dimensional square lattice [14, 15]. Tensor networks have also been applied to tree-like lattices such as the Bethe lattice, also known as the Cayley tree [16, 17]. These are interesting as long range correlations deviate from the mean field polynomially with distance, as opposed to exponentially with DMRG. These networks have proved particularly valuable in quantum chemistry simulations [18, 19, 20].

As well as extending to higher spatial dimensions, tensor networks have included an extra virtual or *holographic* dimension in a similar way to the AdS/CFT correspondence. A simple example is a one dimensional chain of physical sites connected by tree of tensors in a two dimensional space, which would have a structure akin to the graph shown in Figure 1. This extra dimension allows for richer physics to be captured. In such tensor networks, correlations scale as $e^{-\alpha\ell(x_1, x_2)}$, where $\ell(x_1, x_2)$ is the number of tensors that connects leaf x_1 to leaf x_2 [3]. Typical MPS methods for gapped systems give $\ell \approx |x_2 - x_1|$ and correlations scale exponentially. On the other hand, a path length $\ell \approx \log|x_2 - x_1|$ as found in the multi-scale entanglement renormalization ansatz (MERA) [21, 22, 23], leads to a power law decay $\sim e^{-\alpha \log|x_2 - x_1|} \sim |x_2 - x_1|^{-\alpha}$.

Figure 1. A Catalan tree graph with various definitions as defined in the main text. The tree as shown has $n = 15$ and 16 leaves. The indicated separation is $r = 6$ while the associated leaf-to-leaf path length equals $\ell = 6$ as indicated by the thick line. The thick green line denotes the path.

Different quantum systems give rise to different tree structures, and these in turn lead to different distance behaviours for the path lengths. Hence it is interesting to ask more generally about the path lengths of different tree graphs. In a previous work [24], the case of full *and* complete m -ary tree graphs has been studied by using a recursive approach. We found explicit expressions in terms of Hurwitz-Lerch transcendents, as well as numerical results for the incomplete random binary trees. In the present article, we extend our results to the set of all full binary trees (the so-called *Catalan tree graphs*). An example of path lengths in such Catalan trees is given in Figure 1. The absence of paths that would be present in a complete binary tree seems similar to the more random structure seen in random binary trees [24]. We might hence expect that Catalan trees should in many ways be similar to the tree structure found previously [1, 2].

We consider a tree graph where every internal vertex has exactly two children as shown in Figure 1. Such a tree is usually called a *full binary tree*. Let us define n as the number of *internal* vertices in the

graph. We shall refer to such internal vertices as *nodes* or simply *vertices*. The *root* is the top vertex of the tree, which is unique as it is not child of any vertex. We shall call a terminal vertex with no children a *leaf*. The number of full binary trees with n vertices is given by the Catalan number C_n , giving rise to the set being known as the *Catalan tree graphs* [25]. It is straightforward to show that with L denoting the number of leaves, then $L = n + 1$. For the examples given in Figure 2, we see that for $n = 1, 2$, and 3 , we have $C_1 = 1$, $C_2 = 2$, and $C_3 = 5$ unique trees with 2, 3, and 4 leaves in each such tree.

Figure 2. The set of all full binary trees with $n = 1, 2$, and 3 vertices.

2. Generating Functions for Ordered Catalan Trees

2.1. Basic properties of Catalan numbers and the diagrammatic approach

The theory of Catalan numbers and their applications is well-established [26], so we only briefly cite some of the results we shall be needing in the following. Catalan numbers can be computed explicitly using well-known relations such as, e.g.,

$$C_n = \frac{1}{n+1} \binom{2n}{n} = \frac{(2n)!}{(n+1)!n!} = \frac{4n-2}{n+1} C_{n-1} = \sum_{\alpha=0}^{n-1} C_{\alpha} C_{n-\alpha-1}, \quad (1)$$

where the last equation in (2) is a form of Segner's recurrence relation [26]. Alternatively, we can define the C_n 's via generating function as

$$\mathcal{C}(x) = \sum_{n=0}^{\infty} C_n x^n, \quad (2)$$

and, using established notation [27], we write the inverse relation as $C_n = [x^n] \{\mathcal{C}(x)\}$. It is straightforward to show

$$\mathcal{C}(x) = 1 + x\mathcal{C}^2(x), \quad (3)$$

which is the generating function version of Segner's relation and a useful form for subsequent calculations. More algebraic details of generating functions are provided in the Appendix A.1. Next, we introduce a diagrammatic notation [28, 27] for the generating function in which a vertex *represents* x so that we can directly add together diagrams. We begin by setting up a diagrammatic dictionary such that

$$\begin{array}{c} | \\ \triangleq 1 \end{array}, \quad \begin{array}{c} | \\ \diagup \quad \diagdown \\ \triangleq x \end{array}, \quad \begin{array}{c} | \\ \circ \\ \triangleq \mathcal{C}(x) \end{array}. \quad (4)$$

This dictionary allows us to construct a diagrammatic equation for $\mathcal{C}(x)$, i.e.,

$$\begin{aligned} \begin{array}{c} | \\ \circ \end{array} &= \begin{array}{c} | \end{array} + \begin{array}{c} | \\ \diagup \quad \diagdown \end{array} + \begin{array}{c} | \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \end{array} + \begin{array}{c} | \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \quad \diagup \quad \diagdown \end{array} + \begin{array}{c} | \\ \diagup \quad \diagdown \quad \diagup \quad \diagdown \quad \diagup \quad \diagdown \quad \diagup \quad \diagdown \end{array} + \dots \\ &= 1 + x + x^2 + x^2 + x^3 + \dots = 1 + x + 2x^2 + 5x^3 + \dots, \end{aligned} \quad (5)$$

which contains all of the trees shown in Figure 2. We also notice that $\mathcal{C}(x)$ can be generated recursively according to the formula

$$\begin{array}{c} | \\ \circ \end{array} = \begin{array}{c} | \end{array} + \begin{array}{c} | \\ \diagup \quad \diagdown \\ \circ \quad \circ \end{array}. \quad (6)$$

Translating back into algebra, we recover the fundamental relation (3).

3. The Average Depth of Leaves in Catalan trees

Before approaching the problem of average leaf-to-leaf path lengths, we find it necessary to first determine the average depth of a leaf in a Catalan tree. This problem has been studied previously [28], we reconsider it here to establish the notation and introduce our approach.

3.1. External leaf depth

We first consider the simplest case; where the leaf under consideration is the leftmost (or equivalently rightmost). We approach this by finding how many binary trees with n vertices there are such that the leftmost leaf is k vertices away from the root. We will call such a configuration an *external* (because it is on the outer left leaf) *rooted* (because it starts at the root) *path* of length k on a binary tree with n vertices. We also note that due to symmetry reasons the results should hold as well for the *rightmost* leaf of the tree. We will denote by K_{jk} the number of external rooted paths of length k on a binary tree with $n = j + k$ vertices (so that there are always at least k vertices). We also define its generating function as $\mathcal{K}(x, z) = \sum_{jk} K_{jk} x^j z^k$. In order to highlight the path along the leftmost leaves we will define a new diagrammatic dictionary

$$\begin{array}{c} | \\ \vdots \end{array} \triangleq 1, \quad \begin{array}{c} \vdots \\ \diagup \diagdown \end{array} \triangleq x, \quad \begin{array}{c} | \\ \diagdown \end{array} \triangleq z, \quad \begin{array}{c} | \\ \vdots \end{array} \triangleq C(x), \quad \begin{array}{c} | \\ \circ \end{array} \triangleq \mathcal{K}(x, z). \quad (7)$$

Here the z argument allows us to count the number of vertices on (left) external rooted paths while the x term denotes the remaining ones (to the right). The diagrammatic expression for $\mathcal{K}(x, z)$ is then

$$\begin{array}{c} | \\ \circ \end{array} = \begin{array}{c} | \end{array} + \begin{array}{c} | \\ \diagdown \end{array} + \begin{array}{c} | \\ \diagup \diagdown \end{array} + \begin{array}{c} | \\ \diagdown \diagup \end{array} + \begin{array}{c} | \\ \diagup \diagdown \diagup \end{array} + \dots \quad (8)$$

From the results of the previous section we can sum over all of the x vertices to get to

$$\phi = | + \text{ (diagram) } + \text{ (diagram) } + \dots \quad (9)$$

At this point we recognise that the diagrammatic expression (9) is generated by the recursion relation

$$\phi = | + \text{ (diagram) }, \quad (10)$$

which we translate back into algebra according to our diagrammatic dictionary to finally arrive at

$$\mathcal{K}(x, z) = 1 + z\mathcal{C}(x)\mathcal{K}(x, z) = \frac{1}{1 - z\mathcal{C}(x)}. \quad (11)$$

We want to know the average depth of an external leaf on a binary tree with n vertices, e_n . This can be found by calculating the sum of external leaf depths E_n and dividing by the number of possible trees, C_n . We can calculate E_n by multiplying the number of external rooted paths with length k by k and summing as follows:

$$\begin{aligned} E_n &= \sum_{k=1}^n kK_{n-k,k} = \sum_{k=1}^n k[x^{n-k}z^k]\{\mathcal{K}(x, z)\} \\ &= \sum_{k=1}^n [x^{n-k}z^k]\left\{z\frac{\partial}{\partial z}\mathcal{K}(x, z)\right\} = \sum_{k=1}^n [x^{n-k}z^k]\{z\mathcal{C}(x)\mathcal{K}(x, z)^2\} \\ &= [x^n]\{x\mathcal{C}(x)^3\} = C_{n+1} - C_n, \end{aligned} \quad (12)$$

where we have used Equations (3), (A.5), (A.9), (A.11), and (A.13). The average depth e_n is then found to be

$$e_n = \frac{E_n}{C_n} = \frac{C_{n+1}}{C_n} - 1 = \frac{3n}{n+2}, \quad (13)$$

and $e_\infty \equiv \lim_{n \rightarrow \infty} e_n = 3$.

3.2. General leaf depths

Now we generalise the previous result to look at paths which pass through the tree rather than just along the outer edge. We ask how many binary trees with n vertices there are such that the p -th leaf in from the left is m vertices away from the root. We will call this configuration a *rooted path of penetration p* on a binary tree with n vertices. According to this definition, an external rooted path would be a rooted path with penetration $p = 0$. In order to understand the penetration, we need to distinguish between those vertices to the left of the path and those vertices to the right of the path. We will also need to distinguish between those vertices on the path that veer to the left and those that veer to the right.

With this in mind we will construct the generating function $\mathcal{J}(\xi, x, z, \zeta)$ which enumerates those trees containing: (i) i vertices to the left of the path, (ii) j vertices to the right of the path, (iii) k left-turning vertices within the path, and (iv) l right-turning vertices within the path. We will call the series generated $J_{ijkl} = [\xi^i x^j z^k \zeta^l]$ $\{\mathcal{J}(\xi, x, z, \zeta)\}$. Now the diagrammatic method becomes particularly useful. We define the diagrammatic dictionary

$$\begin{array}{l} \begin{array}{c} | \\ \vdots \\ \vdots \end{array} = \begin{array}{c} | \\ \vdots \\ \vdots \end{array} = \begin{array}{c} | \\ \vdots \\ \vdots \end{array} \triangleq 1, \quad \begin{array}{c} | \\ \swarrow \end{array} \triangleq x, \quad \begin{array}{c} | \\ \swarrow \end{array} \triangleq \xi, \quad \begin{array}{c} | \\ \searrow \end{array} \triangleq z, \quad \begin{array}{c} | \\ \searrow \end{array} \triangleq \zeta, \\ \begin{array}{c} \vdots \\ \circ \end{array} \triangleq C(x), \quad \begin{array}{c} \vdots \\ \odot \end{array} \triangleq C(\xi), \quad \begin{array}{c} | \\ \circ \end{array} \triangleq \mathcal{K}(x, z), \quad \begin{array}{c} | \\ \bullet \end{array} \triangleq \mathcal{J}(\xi, x, z, \zeta). \end{array} \quad (14)$$

In advance we can tell that anything happening to the right of the path can be neglected if we replace the edges in the path with external rooted paths. This lets us skip ahead a number of steps and write

$$\bullet = \circ + \begin{array}{c} \circ \\ \diagup \diagdown \\ \bullet \end{array} + \begin{array}{c} \circ \\ \diagup \diagdown \\ \bullet \end{array} + \begin{array}{c} \circ \\ \diagup \diagdown \\ \bullet \end{array} + \begin{array}{c} \circ \\ \diagup \diagdown \\ \bullet \end{array} + \dots \quad (15)$$

With our experience so far we can sum out the ξ vertices, denoting Catalan sub-trees, to get

$$\bullet = \circ + \begin{array}{c} \circ \\ \diagup \diagdown \\ \bullet \end{array} + \begin{array}{c} \circ \\ \diagup \diagdown \\ \bullet \end{array} + \dots, \quad (16)$$

so that we arrive at the recursion relation

$$\bullet = \circ + \begin{array}{c} \circ \\ \diagup \diagdown \\ \bullet \end{array}. \quad (17)$$

We again translate back into algebra and find

$$\mathcal{J}(\xi, x, z, \zeta) = \mathcal{K}(x, z) + \zeta \mathcal{C}(\xi) \mathcal{K}(x, z) \mathcal{J}(\xi, x, z, \zeta) \quad (18)$$

$$= \frac{\mathcal{K}(x, z)}{1 - \zeta \mathcal{C}(\xi) \mathcal{K}(x, z)} = \frac{1}{1 - z \mathcal{C}(x) - \zeta \mathcal{C}(\xi)}. \quad (19)$$

For a path to have penetration p , we need to have i vertices to the left of the path (ξ) and l right turning vertices (ζ) such that $i + l = p$. The way we enforce this is to multiply both ξ and ζ by some dummy variable y within the generating function and then look at the coefficient of y^p in the resulting expansion. Let us therefore define

$$\mathcal{J}^{(p)}(\xi, x, z, \zeta) = [y^p] \{ \mathcal{J}(y\xi, x, z, y\zeta) \} = [y^p] \left\{ \frac{1}{1 - z\mathcal{C}(x) - y\zeta\mathcal{C}(y\xi)} \right\}. \quad (20)$$

From this we can write down the sum of the depths of the p -th leaf (starting from zero) as

$$D_n^{(p)} = \sum_{i+j+k+l=n} (k+l) [\xi^i x^j z^k \zeta^l] [y^p] \{ \mathcal{J}(y\xi, x, z, y\zeta) \}. \quad (21)$$

Exactly as before we can manipulate this expression to bring it into a simpler form using Equations (A.11) and (A.5)

$$D_n^{(p)} = [x^n y^p] \left\{ \frac{1}{[xC(x) + xyC(xy) - 1]} + \frac{1}{[xC(x) + xyC(xy) - 1]^2} \right\}. \quad (22)$$

This is the generating function found by Kirschenhofer [28]. The explicit form is

$$D_n^{(p)} = \frac{2(p+1)(2p+1)(n-p+1)(2n-2p+1)}{(n+1)(n+2)} C_p C_{n-p} - C_n, \quad (23)$$

(cp. Appendix A.2). The average depth of a leaf with penetration p is then

$$d_n^{(p)} = \frac{D_n^{(p)}}{C_n} = \frac{2(p+1)(2p+1)(n-p+1)(2n-2p+1)}{(n+1)(n+2)} \frac{C_p C_{n-p}}{C_n} - 1. \quad (24)$$

We note that a derivation of (24) without the diagrammatic approach is also possible, albeit less adaptable [29].

4. Average Leaf-to-Leaf Path Length in an Ordered Catalan Tree

Our primary task is to calculate the average length of the path separating two leaves on the tree. For convenience in the following derivation we will define the *separation* s as the number of leaves in between the two leaves under consideration. We note that this is one less than the usual definition of distance on a lattice in condensed matter physics (i.e., $s = r - 1$, where $r = |x_2 - x_1|$ if x is the position on the lattice). By this definition adjacent leaves have separation $s = 0$. In

order to enumerate leaf-to-leaf paths with a given separation, it is necessary to distinguish between the left and right arcs of the path following the initial bifurcation. Furthermore we need to distinguish between those vertices sitting between the two arcs of the path and those vertices sitting to the left of the left arc or the right of the right arc. For our purposes, those vertices to the left of the left arc need not be distinguished from those to the right of the right arc. The vertices within an arc need to be separated into those which turn left and those which turn right so our diagrammatic dictionary must contain the following vertices:

$$\begin{array}{ccccccc}
 | & = & || & = & \vdots & = & \vdots \triangleq 1, \\
 & & \swarrow \triangleq z, & & \swarrow \triangleq \zeta, & & \swarrow \triangleq \bar{z}, \\
 & & \searrow \triangleq \bar{\zeta}, & & \searrow \triangleq \bar{\zeta}, & & \searrow \triangleq \bar{\zeta}.
 \end{array} \quad (25a)$$

As yet we have made no reference to those vertices sitting above/outside the initial bifurcation. To account for these we need to extend our diagrammatic dictionary to incorporate the following:

$$\begin{array}{ccc}
 \text{wavy line} & \triangleq 1 & , \\
 \text{wavy line} & \triangleq \lambda & , \\
 \text{wavy line} & \triangleq \mu & .
 \end{array} \quad (25b)$$

The generating function for leaf-to-leaf paths needs to enumerate those trees containing (i) i vertices to the left of the left arc or the right of the right arc, (ii) j vertices to the right of the left arc and the left of the right arc, (iii) k left-turning vertices within the left arc, (iv) l right-turning vertices within the left arc, (v) $\bar{k}$ right-turning vertices within the right arc, (vi) $\bar{l}$ left-turning vertices within the right arc, (vii) m vertices above the initial bifurcation, and (viii) 1 initial bifurcation. The series so generated will be denoted

$$M_{ijkl\bar{k}\bar{l}m} = [\xi^i x^j z^k \zeta^l \bar{z}^{\bar{k}} \bar{\zeta}^{\bar{l}} \lambda^m \mu] \{ \mu \mathcal{M}(\xi, x, z, \zeta, \bar{z}, \bar{\zeta}, \lambda) \}. \quad (26)$$

We will represent the generating function with the diagram

$$\begin{array}{c} \text{diagram} \end{array} \triangleq \mu \mathcal{M}(\xi, x, z, \zeta, \bar{z}, \bar{\zeta}, \lambda) . \quad (27)$$

We begin by writing out the diagrammatic series

$$\begin{array}{l} \text{diagram} = \text{diagram}_1 + \text{diagram}_2 + \text{diagram}_3 + \text{diagram}_4 + \text{diagram}_5 + \text{diagram}_6 + \text{diagram}_7 + \text{diagram}_8 + \text{diagram}_9 \\ + \text{diagram}_{10} + \text{diagram}_{11} + \text{diagram}_{12} + \text{diagram}_{13} + \text{diagram}_{14} + \text{diagram}_{15} + \text{diagram}_{16} + \text{diagram}_{17} + \text{diagram}_{18} \\ + \text{diagram}_{19} + \text{diagram}_{20} + \text{diagram}_{21} + \text{diagram}_{22} + \text{diagram}_{23} + \text{diagram}_{24} + \text{diagram}_{25} + \text{diagram}_{26} \\ + \text{diagram}_{27} + \text{diagram}_{28} + \text{diagram}_{29} + \text{diagram}_{30} + \text{diagram}_{31} + \text{diagram}_{32} + \text{diagram}_{33} + \text{diagram}_{34} \\ + \text{diagram}_{35} + \text{diagram}_{36} + \text{diagram}_{37} + \text{diagram}_{38} + \text{diagram}_{39} + \text{diagram}_{40} + \dots \end{array} \quad (28)$$

We notice that certain diagrams within this series translate to the same term, for example,

$$\text{diagram}_1 = \text{diagram}_2 , \quad (29)$$

so that we ought to write

$$\text{diagram}_1 + \text{diagram}_2 = 2 \times \text{diagram}_1 \times \text{diagram}_2 . \quad (30)$$

Taking this into account, we factorise the generating function such that

$$\begin{aligned} \text{Diagram} &= \left(\zeta + 2 \text{Diagram}_1 + 3 \text{Diagram}_2 + 3 \text{Diagram}_3 + 4 \text{Diagram}_4 + \dots \right) \\ &\times \left(\text{Diagram}_5 + \text{Diagram}_6 + \text{Diagram}_7 + \text{Diagram}_8 + \text{Diagram}_9 + \dots \right). \end{aligned} \quad (31)$$

The second series in parentheses can itself be factorised to give

$$\begin{aligned} \text{Diagram} &= \left(\zeta + 2 \text{Diagram}_1 + 3 \text{Diagram}_2 + 3 \text{Diagram}_3 + 4 \text{Diagram}_4 + \dots \right) \times \text{Diagram}_{10} \\ &\times \left(1 + \text{Diagram}_{11} + \text{Diagram}_{12} + \text{Diagram}_{13} + \text{Diagram}_{14} + \text{Diagram}_{15} + \dots \right) \\ &\times \left(\text{Diagram}_{16} + \text{Diagram}_{17} + \text{Diagram}_{18} + \text{Diagram}_{19} + \text{Diagram}_{20} + \text{Diagram}_{21} + \dots \right). \end{aligned} \quad (32)$$

The latter two series in parentheses we recognise as the generating functions (19) of rooted paths on the left and right arcs, respectively. So let us write

$$\text{Diagram}_{11} = \mathcal{J}(\xi, x, z, \zeta) \quad , \quad \text{Diagram}_{16} = \mathcal{J}(\xi, x, \bar{z}, \bar{\zeta}) \quad , \quad (33)$$

using which we have

$$\text{Diagram} = \left(\zeta + 2 \text{Diagram}_1 + 3 \text{Diagram}_2 + 3 \text{Diagram}_3 + 4 \text{Diagram}_4 + \dots \right) \times \text{Diagram}_{10} \times \text{Diagram}_{16}. \quad (34)$$

The remaining series left to be summed can be seen to be $\sum_n (n+1)C_n \lambda^n$

which we can write as $\frac{\partial}{\partial \lambda} \lambda \mathcal{C}(\lambda)$. Altogether we find for the generating function

$$\mu \mathcal{M}(\xi, x, z, \zeta, \bar{z}, \bar{\zeta}, \lambda) = \mu \mathcal{J}(\xi, x, z, \zeta) \times \mathcal{J}(x, \xi, \bar{z}, \bar{\zeta}) \times \frac{\partial}{\partial \lambda} [\lambda \mathcal{C}(\lambda)]. \quad (35)$$

The derivative of $\mathcal{C}(\lambda)$ can be easily determined given (3), which yields

$$\begin{aligned} \frac{\partial}{\partial \lambda} \mathcal{C}(\lambda) &= \mathcal{C}(\lambda)^2 + 2\lambda \mathcal{C}(\lambda) \frac{\partial}{\partial \lambda} \mathcal{C}(\lambda) = \frac{\mathcal{C}(\lambda)^2}{1 - 2\lambda \mathcal{C}(\lambda)} \quad \text{and} \quad \frac{\partial}{\partial \lambda} [\lambda \mathcal{C}(\lambda)] = \mathcal{C}(\lambda) + \\ &\frac{\lambda \mathcal{C}(\lambda)^2}{1 - 2\lambda \mathcal{C}(\lambda)} = \frac{\mathcal{C}(\lambda) - \lambda \mathcal{C}(\lambda)^2}{1 - 2\lambda \mathcal{C}(\lambda)}. \end{aligned}$$

Finally, we arrive at the generating

function

$$\mathcal{M}(\xi, x, z, \zeta, \bar{z}, \bar{\zeta}, \lambda) = \frac{1}{1 - z\mathcal{C}(x) - \zeta\mathcal{C}(\xi)} \frac{1}{1 - \bar{z}\mathcal{C}(x) - \bar{\zeta}\mathcal{C}(\xi)} \frac{1}{1 - 2\lambda \mathcal{C}(\lambda)}. \quad (36)$$

The separation between the two leaves is given by the number of vertices (x) sitting between the two arcs of the path plus the number of left-turning vertices (z) in the left arc of the path plus the number of right-turning vertices ($\bar{z}$) in the right arc of the path. With this in mind we attach a dummy variable to these variables and look for coefficients of y^s , giving

$$M^{(s)}(\xi, x, z, \zeta, \bar{z}, \bar{\zeta}, \lambda) = [y^s] \mathcal{M}(\xi, yx, yz, \zeta, y\bar{z}, \bar{\zeta}, \lambda, \mu). \quad (37)$$

To find the average length of a path between leafs with separation s we first need to sum over all trees with n vertices, the number of paths with length $k + l + \bar{k} + \bar{l} + 1$ multiplied by that length. The factor of 1 here comes in because we always need to account for the initial bifurcation given by the μ vertex. We therefore define

$$S_n^{(s)} = \sum_{i+j+k+l+\bar{k}+\bar{l}+m+1=n} (k + l + \bar{k} + \bar{l} + 1) M_{ijkl\bar{k}\bar{l}m}^{(s)}. \quad (38)$$

We proceed to manipulate this expression in a similar manner to Equation (12). First using (A.11) we simplify the summand

$$\begin{aligned}
& (k + l + \bar{k} + \bar{l} + 1) M_{ijkl\bar{k}\bar{l}m}^{(s)} \\
&= (k + l + \bar{k} + \bar{l} + 1) [\xi^i x^j z^k \zeta^l \bar{z}^{\bar{k}} \bar{\zeta}^{\bar{l}} \lambda^m y^s] \{ \mathcal{M}(\xi, yx, yz, \zeta, y\bar{z}, \bar{\zeta}, \lambda) \} \\
&= [\xi^i x^j z^k \zeta^l \bar{z}^{\bar{k}} \bar{\zeta}^{\bar{l}} \lambda^m y^s] \\
&\quad \left\{ \left(z \frac{\partial}{\partial z} + \bar{z} \frac{\partial}{\partial \bar{z}} + \zeta \frac{\partial}{\partial \zeta} + \bar{\zeta} \frac{\partial}{\partial \bar{\zeta}} + 1 \right) \mathcal{M}(\xi, yx, yz, \zeta, y\bar{z}, \bar{\zeta}, \lambda) \right\}, \quad (39)
\end{aligned}$$

to which the derivatives can be performed straightforwardly,

$$\begin{aligned}
& \left(z \frac{\partial}{\partial z} + \bar{z} \frac{\partial}{\partial \bar{z}} + \zeta \frac{\partial}{\partial \zeta} + \bar{\zeta} \frac{\partial}{\partial \bar{\zeta}} + 1 \right) \mathcal{M}(\xi, yx, yz, \zeta, y\bar{z}, \bar{\zeta}, \lambda) \\
&= \frac{1}{1 - 2\lambda\mathcal{C}(\lambda)} \frac{1}{1 - yz\mathcal{C}(yx) - \zeta\mathcal{C}(\xi)} \frac{1}{1 - y\bar{z}\mathcal{C}(yx) - \bar{\zeta}\mathcal{C}(\xi)} \\
&\quad \times \left[\frac{yz\mathcal{C}(yx) + \zeta\mathcal{C}(\xi)}{1 - yz\mathcal{C}(yx) - \zeta\mathcal{C}(\xi)} + \frac{y\bar{z}\mathcal{C}(yx) + \bar{\zeta}\mathcal{C}(\xi)}{1 - y\bar{z}\mathcal{C}(yx) - \bar{\zeta}\mathcal{C}(\xi)} + 1 \right]. \quad (40)
\end{aligned}$$

Applying the formula (A.5) to $\xi, x, z, \bar{z}, \zeta, \bar{\zeta}$, and λ , $S_n^{(s)}$ is reduced to

$$S_n^{(s)} = [x^{n-1} y^s] \left\{ \frac{1}{1 - 2x\mathcal{C}(x)} \left[\frac{2[x\mathcal{C}(x) + xy\mathcal{C}(xy)]}{[1 - x\mathcal{C}(x) - xy\mathcal{C}(xy)]^3} + \frac{1}{[1 - x\mathcal{C}(x) - xy\mathcal{C}(xy)]^2} \right] \right\}. \quad (41)$$

Simplifying slightly using (A.9) we arrive at

$$S_n^{(s)} = [x^n y^s] \left\{ \frac{1}{1 - 2x\mathcal{C}(x)} \frac{1}{[1 - x\mathcal{C}(x) - xy\mathcal{C}(xy)]^2} \left[\frac{2}{1 - x\mathcal{C}(x) - xy\mathcal{C}(xy)} - 1 \right] \right\}. \quad (42)$$

This summed length with separation s on a tree with n vertices can be further simplified as follows:

$$\begin{aligned}
 S_n^{(s)} &= [x^{n-1}y^s] \left\{ \left[\frac{2}{[1 - x\mathcal{C}(x) - xy\mathcal{C}(xy)]^3} - \frac{1}{[1 - x\mathcal{C}(x) - xy\mathcal{C}(xy)]^2} \right] \frac{\partial x\mathcal{C}(x)}{\partial x} \right\} \\
 &= [x^{n-1-s}z^s] \left\{ \left[\frac{2}{[1 - x\mathcal{C}(x) - z\mathcal{C}(z)]^3} - \frac{1}{[1 - x\mathcal{C}(x) - z\mathcal{C}(z)]^2} \right] \frac{\partial x\mathcal{C}(x)}{\partial x} \right\} \\
 &= [x^{n-1-s}z^s] \left\{ \frac{\partial}{\partial x} \left[\frac{1}{[1 - x\mathcal{C}(x) - z\mathcal{C}(z)]^2} - \frac{1}{[1 - x\mathcal{C}(x) - z\mathcal{C}(z)]} \right] \right\} \\
 &= (n-s)[x^n y^s] \left\{ \frac{1}{[1 - x\mathcal{C}(x) - xy\mathcal{C}(xy)]^2} - \frac{1}{[1 - x\mathcal{C}(x) - xy\mathcal{C}(xy)]} \right\}, \quad (43)
 \end{aligned}$$

where we have used $z = xy$. By comparison with Equation (22), we conclude that the summed length of leaf to leaf paths is related directly to the sum of the depth of the leaves by

$$S_n^{(s)} = (n-s)D_n^{(s)}, \quad (44)$$

and hence the *average* length of a leaf to leaf path with separation s on a tree with n vertices is

$$\ell_n^{(s)} = \frac{(n-s)D_n^{(s)}}{(n-s)C_n} = \frac{D_n^{(s)}}{C_n} = d_n^{(s)}. \quad (45)$$

We therefore see that the path length when averaged over both the set of all trees as well as the all pairs of leaves with separation s within each tree is identical to the average depth of a rooted path with penetration s . The explicit form of which is given by Equation (24).

The asymptotic properties of the path length in the limit of large n can be found using Stirling's approximation

$$n! \sim \sqrt{2\pi n} \left(\frac{n}{e} \right)^n. \quad (46)$$

Accordingly, we find that $C_n \sim \frac{1}{\sqrt{\pi}} \frac{1}{n\sqrt{n}} 2^{2n}$ for large n . Therefore, we conclude from Equation (24) that

$$\ell_\infty^{(s)} \equiv \lim_{n \rightarrow \infty} \ell_n^{(s)} = \frac{(s+1)(2s+1)}{4^{s-1}} C_{s-1}.$$

In the continuum limit, $0 \ll s \ll n$, we have

$$\ell_\infty^{(s)} \sim \sqrt{\frac{64s}{\pi}}. \quad (47)$$

In Figure 3, we transform back into an expression for $r = s + 1$, $\ell_n(r)$, to compare with previous results for the complete binary tree [24], shown as a dashed line. We show the average path length for various separations as well as the large n limit. This clearly illustrates that the different tree geometry can dramatically change the scaling of the path length.

Figure 3. Average length of a leaf to leaf path $\ell_n(r)$ versus separation r for small $n = 50$ (solid black line), 100 (solid red), 200 (solid blue) and large $n = 5,000$ (dashed black line), 10,000 (dashed red), 20,000 (dashed blue). The solid green line denotes $\ell_\infty(r)$, the dotted line corresponds to r while the dashed-dotted line shows the corresponding result for complete binary trees [24].

5. Conclusion

In summary, we computed the average leaf-to-leaf path length on ordered Catalan trees with n nodes using a diagrammatic method for the generating functions. After completion of our work, we were made aware of a proof of the average depth of a leaf of penetration p (Equation (24)) by Kirschenhofer [28] and a later generalisation to all statistical moments [30]. As the leaf depths and path lengths are directly related via the rerooting invariance of a tree to a random vertex (particularly, rerooting at the k -th leaf) [32], the results of [30] for the higher statistical moments should also be valid here. Certainly, one advantage

of the explicitly constructive approach¹ used here is the availability of intermediate results such as Equations (12), (23), and (24), which can be important when implementing numerical algorithms as in [1, 2]. Moreover, we believe that the diagrammatic approach can also be employed to calculate the statistical moments of the leaf-to-leaf distances when distinct paths, and/or trees, are weighted differently (e.g., drawn from a particular distribution).

The final results for $\ell_n(r)$ and $\ell_\infty(r)$ are quite surprising when comparing, as done in Figure 3, with the corresponding expressions $\mathcal{L}_n(r)$ and $\mathcal{L}_\infty(r)$ for complete binary trees [24] and the tree graphs emerging from the tree tensor network [1]. We find that the ℓ -path lengths take larger values than the $\mathcal{L}$'s. This can be rationalized as follows: in order for n vertices to form into a complete binary graph, those vertices are very densely *packed*, hence giving rise to a small $\mathcal{L}_n(r)$. On the other hand, Catalan graphs with n vertices can have a much more extended structure, leading to larger path lengths $\ell_n(r)$ for the same r . Comparing to the tree tensor networks, this result shows that our naive expectation expressed in the introduction, is wrong: the path lengths are quite different for larger r values and hence the implied correlation functions have a very different long distance behaviour. Just as for complete binary graphs, it remains to be seen what Hamiltonians, if any, correspond to these correlations.

Acknowledgements

We thank the EPSRC for financial support (EP/J003476/1) and provision of computing resources through the MidPlus Regional HPC Centre (EP/K000128/1). We are grateful to H. Prodinger for pointing out relevant references [28, 31, 30]. UK data statement: No new data was generated in this research.

¹An alternative algebraic derivation of (45) can be found in [29].

References

- [1] A. M. Goldsborough and R. A. Römer, Self-assembling tensor networks and holography in disordered spin chains, *Phys. Rev. B* 89(21) (2014), Article 214203.
DOI: <https://doi.org/10.1103/PhysRevB.89.214203>
- [2] A. M. Goldsborough and G. Evenbly, Entanglement renormalization for disordered systems, *Phys. Rev. B* 96(15) (2017), Article 155136.
DOI: <https://doi.org/10.1103/PhysRevB.96.155136>
- [3] G. Evenbly and G. Vidal, Tensor network states and geometry, *J. Stat. Phys.* 145(4) (2011), 891-918.
DOI: <https://doi.org/10.1007/s10955-011-0237-4>
- [4] B. Swingle, Entanglement renormalization and holography, *Phys. Rev. D* 86(6) (2012), Article 065007.
DOI: <https://doi.org/10.1103/PhysRevD.86.065007>
- [5] J. Molina-Vilaplana, Holographic geometries of one-dimensional gapped quantum systems from tensor network states, *J. High Energy Phys.* 2013, (2013), 1-25.
DOI: [https://doi.org/10.1007/JHEP05\(2013\)024](https://doi.org/10.1007/JHEP05(2013)024)
- [6] J. Maldacena, The large-N limit of superconformal field theories and supergravity, *Int. J. Theor. Phys.* 38(4) (1999), 1113-1133.
DOI: <https://doi.org/10.1023/A:1026654312961>
- [7] J. McGreevy, Holographic duality with a view toward many-body physics, *Adv. High Energy Phys.* (2010) Article ID 723105, 54 pages.
DOI: <http://dx.doi.org/10.1155/2010/723105>
- [8] K. H. Rosen, *Discrete Mathematics and its Applications*, Seventh Edition, McGraw Hill, New York, NY, 2012.
- [9] R. Orús, A practical introduction to tensor networks: Matrix product states and projected entangled pair states, *Ann. Phys.* 349 (2014), 117-158.
DOI: <https://doi.org/10.1016/j.aop.2014.06.013>
- [10] R. Orús, Advances on tensor network theory: Symmetries, fermions, entanglement, and holography, *Eur. Phys. J. B* 87(11) (2014), 280.
DOI: <https://doi.org/10.1140/epjb/e2014-50502-9>
- [11] S. R. White, Density matrix formulation for quantum renormalization groups, *Phys. Rev. Lett.* 69(19) (1992), 2863-2866.
DOI: <https://doi.org/10.1103/PhysRevLett.69.2863>
- [12] S. Östlund and S. Rommer, Thermodynamic limit of density matrix renormalization, *Phys. Rev. Lett.* 75(19) (1995), 3537-3540.
DOI: <https://doi.org/10.1103/PhysRevLett.75.3537>

- [13] U. Schollwöck, The density-matrix renormalization group in the age of matrix product states, *Ann. Phys.* 326(1) (2011), 96-192.
DOI: <https://doi.org/10.1016/j.aop.2010.09.012>
- [14] F. Verstraete and J. I. Cirac, Renormalization algorithms for quantum-many body systems in two and higher dimensions, *arXiv:cond-mat/0407066* (2004).
- [15] F. Verstraete, V. Murg and J. I. Cirac, Matrix product states, projected entangled pair states, and variational renormalization group methods for quantum spin systems, *Adv. Phys.* 57(2) (2008), 143-224.
DOI: <https://doi.org/10.1080/14789940801912366>
- [16] V. Murg et al., Simulating strongly correlated quantum systems with tree tensor networks, *Phys. Rev. B* 82(20) (2010), Article 205105.
DOI: <https://doi.org/10.1103/PhysRevB.82.205105>
- [17] K. Gunst et al., T3NS: Three-legged tree tensor network states, *arXiv:1801.09998* (2018).
- [18] N. Nakatani and G. K.-L. Chan, Efficient tree tensor network states (TTNS) for quantum chemistry: Generalizations of the density matrix renormalization group algorithm, *J. Chem. Phys.* 138(13) (2013), Article 134113.
DOI: <https://doi.org/10.1063/1.4798639>
- [19] S. Szalay et al., Tensor product methods and entanglement optimization for *ab initio* quantum chemistry, *Int. J. Quantum Chem.* 115(19) (2015), 1342-1391.
DOI: <https://doi.org/10.1002/qua.24898>
- [20] V. Murg et al., Tree tensor network state with variable tensor order: An efficient multireference method for strongly correlated systems, *J. Chem. Theory Comput.* 11(3) (2015), 1027-1036.
DOI: <http://dx.doi.org/10.1021/ct501187j>
- [21] G. Vidal, Entanglement renormalization, *Phys. Rev. Lett.* 99(22) (2007), Article 220405.
DOI: <https://doi.org/10.1103/PhysRevLett.99.220405>
- [22] G. Vidal, Class of quantum many-body states that can be efficiently simulated, *Phys. Rev. Lett.* 101(11) (2008), Article 110501.
DOI: <https://doi.org/10.1103/PhysRevLett.101.110501>
- [23] G. Evenbly and G. Vidal, Algorithms for entanglement renormalization, *Phys. Rev. B* 79(14) (2009), Article 144108.
DOI: <https://doi.org/10.1103/PhysRevB.79.144108>
- [24] A. M. Goldsborough, S. A. Rautu and R. A. Römer, Leaf-to-leaf distances and their moments in finite and infinite ordered m -ary tree graphs, *Phys. Rev. E* 91(4) (2015), Article 042133.
DOI: <https://doi.org/10.1103/PhysRevE.91.042133>

- [25] R. Sedgewick and P. Flajolet, *An Introduction to the Analysis of Algorithms*, Addison-Wesley, Westford, MA, Second Edition, 2013.
- [26] T. Koshy, *Catalan Numbers with Applications*, Oxford University Press, Oxford, Second Edition, 2009.
- [27] H. S. Wilf, *Generating Functionology*, Academic Press, London, Second Edition, 1994.
- [28] P. Kirschenhofer, On the height of leaves in binary trees, *J. Comb. Inform. System Sci.* 8 (1983), 44-60.
- [29] A. M. Goldsborough et al., Leaf-to-leaf distances in ordered Catalan tree graphs, *arXiv:1502.07893v1 [math-ph]* (2015).
- [30] A. Panholzer and H. Prodinger, Moments of level numbers of leaves in binary trees, *J. Stat. Plan. Inference* 101(1-2) (2002), 267-279.

DOI: [https://doi.org/10.1016/S0378-3758\(01\)00187-2](https://doi.org/10.1016/S0378-3758(01)00187-2)

- [31] P. Kirschenhofer, Some new results on the average height of binary trees, *Ars Combinatoria* 16A (1983), 255-260.
- [32] B. Haas, J. Pitman and M. Winkel, Spinal partitions and invariance under re-rooting of continuum random trees, *Ann. Probab.* 37(4) (2009), 1381-1411.

DOI: <http://dx.doi.org/10.1214/08-AOP434>

A. Appendix

A.1. More on generating functions

We make extensive use of generating functions [26, 27] as they offer a convenient way to manipulate relations between the set of Catalan numbers. More generally, they serve as a very useful formal device for manipulating a series and for determining the properties of unknown series [27]. Given a general (infinite) series $a_0, a_1, a_2, a_3, \dots$, it is always possible to formally define a function

$$a(x) = a_0 + a_1x + a_2x^2 + a_3x^3 + \dots = \sum_{n=0}^{\infty} a_n x^n, \quad (\text{A.1})$$

which we call the *generating function* of the sequence a_n . We can also invert the above definition and instead say that a_n is the coefficient of x^n in the Taylor series representation of $a(x)$ about zero. We employ the notation [27] $a_n = [x^n] \{a(x)\}$. For example, squaring (2) gives,

$$\begin{aligned} \mathcal{C}^2(x) &= C_0^2 + (C_0C_1 + C_1C_0)x + \dots + (C_0C_n + C_1C_{n-1} + \dots + C_nC_0)x^n + \dots \\ &= C_1 + C_2x + C_3x^2 + \dots + C_{n+1}x^n + \dots = \frac{\mathcal{C}(x) - C_0}{x}, \end{aligned} \quad (\text{A.2})$$

and we have used the final part of Equation (1) in each term. Multiplication by x results in (3).

Below, we list some particular generating functions and their associated series coefficients. The series coefficients of $a(x)$ can be expressed as [27]

$$[x^n] \{a(x)\} = \frac{1}{n!} \left. \frac{\partial^n a(x)}{\partial x^n} \right|_{x=0} = \oint \frac{dx}{2\pi i} \frac{1}{x} \frac{a(x)}{x^n}. \quad (\text{A.3})$$

A useful identity is the *Lagrange inversion formula* [27, 25]: Suppose u is a function which can be expressed as $u(x) = x\phi(u)$ where the function ϕ satisfies $\phi(0) = 1$, then for a given function f , we have

$$[x^n] \{f(u(x))\} = \frac{1}{n} [u^{n-1}] \{f'(u)\phi(u)^n\}. \quad (\text{A.4})$$

Generating functions can also be defined for multi-indexed series $a_{ijk\dots}$ [27]. We will extend our notation so that

$[x_1^{n_1} x_2^{n_2} \dots x_r^{n_r}] \{f(x_1, x_2, \dots, x_r)\}$ is the coefficient of $x_1^{n_1} x_2^{n_2} \dots x_r^{n_r}$ in the Taylor series of $f(x_1, x_2, \dots, x_r)$. A convenient identity for dealing with generating functions of many variables is

$$\sum_{r=0}^n [x^r y^{n-r}] \{a(x, y)\} = [x^n] \{a(x, y)\}. \quad (\text{A.5})$$

As an example of the use of the notation for generating functions, [27] we list some particular generating functions and their associated series coefficients,

$$[x^n] \{x^p\} = \delta_{n,p}, [x^n] \{e^x\} = 1/n!, [x^n] \left\{ \frac{1}{1-x} \right\} = 1, [x^n] \{(1+x)^p\} = \binom{p}{n}. \quad (\text{A.6})$$

If $[x^n] \{a(x)\} = a_n$ and $[x^n] \{b(x)\} = b_n$, one finds

$$[x^n] \{a(x)b(x)\} = \sum_{k=0}^n a_k b_{n-k}. \quad (\text{A.7})$$

Raising and lowering of indices in series coefficients can be achieved using

$$[x^{n-1}] \{a(x)\} = [x^n] \{xa(x)\}, \quad (\text{A.8})$$

$$[x^{n+1}] \{a(x)\} = [x^n] \left\{ \frac{a(x) - a(0)}{x} \right\}. \quad (\text{A.9})$$

Differentiating Equation (A.1) we notice that

$$[x^n] \left\{ \frac{\partial a(x)}{\partial x} \right\} = n[x^{n+1}] \{a(x)\}, \quad (\text{A.10})$$

combining this with Equation (A.8) we get the useful relation

$$n[x^n] \{a(x)\} = [x^n] \left\{ x \frac{\partial}{\partial x} a(x) \right\}. \quad (\text{A.11})$$

From the series definition it should be clear that constant multiples of the argument can just be brought out front as follows

$$[x^n] \{a(cx)\} = c^n [x^n] \{a(x)\}. \quad (\text{A.12})$$

For Equation (12), it is useful to notice that, using (3),

$$\mathcal{K}(x, x) = \mathcal{C}(x), \quad \frac{\partial \mathcal{K}(x, z)}{\partial z} = \mathcal{C}(x) \mathcal{K}(x, z)^2. \quad (\text{A.13})$$

A.2. Derivation of the average depth of a leaf

Equation (22) can be simplified by multiplying top and bottom by $x\mathcal{C}(x) - xy\mathcal{C}(xy)$, due to $1/[1 - x\mathcal{C}(x) - xy\mathcal{C}(xy)] = [x\mathcal{C}(x) - xy\mathcal{C}(xy)]/(x - xy)$.

This allows us to bring the generating function for the summed lengths into the simple form

$$D_n^{(p)} = [x^n y^p] \left\{ \frac{\mathcal{C}(x) - y\mathcal{C}(xy)}{1 - y} \left[\frac{\mathcal{C}(x) - y\mathcal{C}(xy)}{1 - y} - 1 \right] \right\}. \quad (\text{A.14})$$

By applying the identity (A.12), we can begin to evaluate the coefficient of x^n in this generating function,

$$\begin{aligned}
 D_n^{(p)} &= [x^n y^p] \left\{ \frac{1}{(1-y)^2} [\mathcal{C}(x)^2 + y^2 \mathcal{C}(xy)^2 - 2y \mathcal{C}(x) \mathcal{C}(xy)] - \frac{1}{1-y} [\mathcal{C}(x) - y \mathcal{C}(xy)] \right\} \\
 &= [y^p] \left\{ \frac{1}{(1-y)^2} [[x^n] \{\mathcal{C}(x)^2\} + y^2 y^n [x^n] \{\mathcal{C}(x)^2\} - 2y [x^n] \{\mathcal{C}(x) \mathcal{C}(xy)\}] \right. \\
 &\quad \left. - \frac{1}{1-y} [[x^n] \{\mathcal{C}(x)\} - y y^n [x^n] \{\mathcal{C}(x)\}] \right\} \\
 &= [y^p] \left\{ \frac{1+y^{n+2}}{(1-y)^2} C_{n+1} - \frac{1+y^{n+1}}{1-y} C_n - \frac{2y}{(1-y)^2} [x^n] \{\mathcal{C}(x) \mathcal{C}(xy)\} \right\},
 \end{aligned} \tag{A.15}$$

the final term here can be evaluated using (A.7). We also notice here that p is always less than n (there is no way a path can contain more vertices than the tree it runs through) so we can omit the terms containing y^n . We recognise that $[y^p] \{(1-y)^{-2}\} = (p+1)$, therefore

$$\begin{aligned}
 D_n^{(p)} &= (p+1)C_{n+1} - C_n - 2[y^p] \left\{ \frac{y}{(1-y)^2} \sum_{k=0}^n C_{n-k} y^k C_k \right\} \\
 &= (p+1)C_{n+1} - C_n - 2[y^p] \left\{ \sum_{k=0}^n \frac{y^{k+1}}{(1-y)^2} C_k C_{n-k} \right\}.
 \end{aligned} \tag{A.16}$$

The sum in the final term here contains powers of y running up to $n+1$. Restricting to terms with powers of $y \leq p$, the summation becomes

$$\begin{aligned}
 D_n^{(p)} &= (p+1)C_{n+1} - C_n - 2 \sum_{k=0}^{p-1} [y^p] \left\{ \frac{y^{k+1}}{(1-y)^2} \right\} C_k C_{n-k} \\
 &= (p+1)C_{n+1} - C_n - 2 \sum_{k=0}^{p-1} [y^{p-k-1}] \left\{ \frac{1}{(1-y)^2} \right\} C_k C_{n-k}.
 \end{aligned} \tag{A.17}$$

We arrive at an expression for the summed length of paths from the root to the p -th leaf in a binary tree with n vertices.

$$D_n^{(p)} = (p+1)C_{n+1} - C_n - 2 \sum_{k=0}^{p-1} (p-k)C_k C_{n-k}. \quad (\text{A.18})$$

In order to reach a closed formula we need to remove the final sum, which is similar to Segner's relation $\sum_{k=0}^n C_k C_{n-k} = C_{n+1}$ but with an incomplete sum, i.e.,

$$s_{pn} = \sum_{k=0}^p C_k C_{n-k}. \quad (\text{A.19})$$

We claim that

$$s_{pn} = \frac{1}{2} C_{n+1} + \frac{1}{2} \frac{(2p+1-n)(p+2)(n-p+1)}{(n+1)(n+2)} C_{p+1} C_{n-p}, \quad (\text{A.20})$$

which may be proven by induction, using only the recurrence relation for the Catalan numbers given in (1). First we confirm validity for $p = 0$, i.e.,

$$\begin{aligned} s_{0n} &= \frac{1}{2} C_{n+1} + \frac{1}{2} \frac{(1-n)(2)(n+1)}{(n+1)(n+2)} C_1 C_n = \frac{2n+1}{n+2} C_n + \frac{(1-n)}{(n+2)} C_n \\ &= C_n = \sum_{k=0}^0 C_k C_{n-k}. \end{aligned} \quad (\text{A.21})$$

Assuming the expression to be valid for p , we proceed to show that this implies the validity for $p+1$, i.e.,

$$\begin{aligned} s_{p+1,n} &= s_{pn} + C_{p+1} C_{n-(p+1)} \\ &= \frac{1}{2} C_{n+1} + \left[\frac{1}{2} \frac{(2p+1-n)(p+2)(n-p+1)}{(n+1)(n+2)} C_{n-p} + C_{n-p-1} \right] C_{p+1} \\ &= \frac{1}{2} C_{n+1} + \left[\frac{(2p+1-n)(p+2)(2(n-p)-1)}{(n+1)(n+2)} C_{n-p-1} + C_{n-p-1} \right] C_{p+1} \end{aligned}$$

$$\begin{aligned}
 &= \frac{1}{2} C_{n+1} + \frac{(2p+3-n)(n-p)(2p+3)}{(n+1)(n+2)} C_{n-p-1} + C_{p+1} \\
 &= \frac{1}{2} C_{n+1} + \frac{(2p+3-n)(n-p)(2p+3)}{(n+1)(n+2)} C_{n-p-1} \frac{1}{2} \frac{p+3}{2p+3} C_{p+1} \\
 &= \frac{1}{2} C_{n+1} + \frac{1}{2} \frac{[2(p+1)+1-n][(p+1)+2][n-(p+1)+1]}{(n+1)(n+2)} C_{n-(p+1)} C_{p+1},
 \end{aligned} \tag{A.22}$$

and so the formula is proven by induction. As a final check we can look at the complete sum s_{nn} which should reproduce Segner's relation

$$\begin{aligned}
 s_{nn} &= \frac{1}{2} C_{n+1} + \frac{1}{2} \frac{(2n+1-n)(n+2)(n-n+1)}{(n+1)(n+2)} C_{n+1} C_{n-n} \\
 &= \frac{1}{2} C_{n+1} + \frac{1}{2} C_{n+1} C_1 = C_{n+1}. \tag{A.23}
 \end{aligned}$$

Similarly, the relation

$$\begin{aligned}
 \sum_{k=0}^{p-1} (p-k) C_{n-k} C_k &= \frac{1}{(n+1)(n+2)} \{ (2n+1)(p+1)(n+1) C_n \\
 &\quad - (2p+1)(p+1) C_p [2(n-p)+1] (n-p+1) C_{n-p} \},
 \end{aligned} \tag{A.24}$$

can be proven by induction. Finally, using (A.24), we find that (A.18) in explicit form gives the depth function (24).