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Central limit theorem for the bifurcation ratio of a random binary tree

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Abstract

In order to formulate and examine the central limit theorem for a binary tree numerically, a method for generating random binary trees is presented. We first propose the correspondence between binary trees and a certain type of binary sequences (which we call Dyck sequences). Then, the method for generating random Dyck sequences is shown. Also, we propose the method of branch ordering of a binary tree by means of only the corresponding Dyck sequence. We confirm that the method is in good consistency with the topological analysis of binary trees known as the Horton–Strahler analysis. Two types of central limit theorem are numerically confirmed, and the obtained results are expressed in simple forms. Furthermore, the proposed method is available for a wide range of the topological analysis of binary trees.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Branching patterns are widely spread in Nature [1, 2]. Some patterns appear to be quite similar to each other even if their generation process is different. The branching patterns are characterized from various standpoints. For example, a property related to spatial configurations is called geometric, including length, spatial symmetry and fractality. On the other hand, a property based on the graph-theoretic structure (and not on spatial extent) is called topological. Connectivity and degree distributions of complex networks are typical and important topological structures. In particular, the topological structure of a branching pattern can be expressed by a binary-tree graph.

A *full binary tree* is a tree graph (i.e. a connected graph without loops) where every node has exactly zero or two 'children' (see figure 1 for reference). For simplicity, we use the term 'binary tree' instead of 'full binary tree' hereafter, since we focus on only full binary trees throughout the paper. A node without any children is called a *leaf*, a node without 'parents' is called a *root* and the number of leaves is called the *magnitude*. Binary trees have been

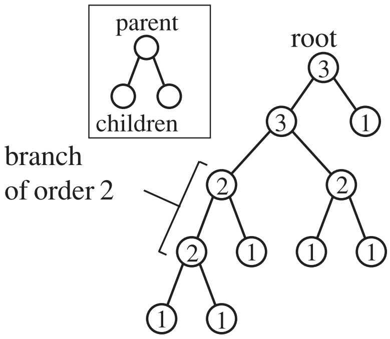

Figure 1. An example of a binary tree of magnitude 6. The numbers on the nodes represent their orders.

investigated mainly in computer science, and frequently used in order to represent some types of data structures such as binary search trees, binary heaps and expression trees [3, 4].

In order to derive topological characteristics of branching patterns, a method of branch ordering has been introduced by Horton [5] and Strahler [6] (known as the *Horton–Strahler analysis*). The method can measure the ramification complexity and the hierarchical structure of branching patterns. For each node v in a binary tree T, the *Horton–Strahler index* (or *order*) $S(v)$ is defined recursively as

$$S(v) = \begin{cases} 1, & \text{if } v \text{ is a leaf,} \\ \max\{S(v_1), S(v_2)\} + \delta_{S(v_1),S(v_2)}, & \text{if } v_1 \text{ and } v_2 \text{ are the children of } v, \end{cases} \tag{1}$$

where $\delta_{i,j}$ is the Kronecker delta. We use 'order' for individual nodes, and the 'Horton–Strahler index' for the whole set of nodes. We define a *branch* of order r as a maximal path connecting nodes of order r. The ratio of the number of branches of two subsequent orders is called the *bifurcation ratio*, and it has been found in many branching patterns that the bifurcation ratio takes an almost constant value for different orders, which is known as 'Horton's law of stream numbers' especially in river networks [5]. Horton–Strahler analysis has been applied to a wide range of branching patterns [7–15].

A simple model called the *random model* or the *equiprobable model*, formulated by Shreve [16], is a finite probability space (Ω_n, P_n), where Ω_n denotes the sample space consisting of topologically distinct binary trees of magnitude n, and P_n is the uniform probability measure on Ω_n. We also introduce a random variable $S_{r,n} : \Omega_n \to \mathbb{N} \cup \{0\}$ such that $S_{r,n}(T)$ represents the number of branches of order r in a binary tree $T \in \Omega_n$. Horton's law on (Ω_n, P_n) is stated in the form

$$\frac{E(S_{r,n})}{E(S_{r-1,n})} \to \frac{1}{4} \qquad \text{as} \quad n \to \infty, \tag{2}$$

where $E(\cdot)$ denotes the average on (Ω_n, P_n), and $r = 2, 3, \ldots$. The analytical or combinatorial properties of $S_{r,n}$ are discussed in [17–23] for example.

Wang and Waymire [24] analytically proved the central limit theorem

$$\sqrt{n}\left(\frac{S_{2,n}}{n} - \frac{1}{4}\right) \Rightarrow N\left(0, \frac{1}{16}\right) \qquad \text{as} \quad n \to \infty, \tag{3}$$

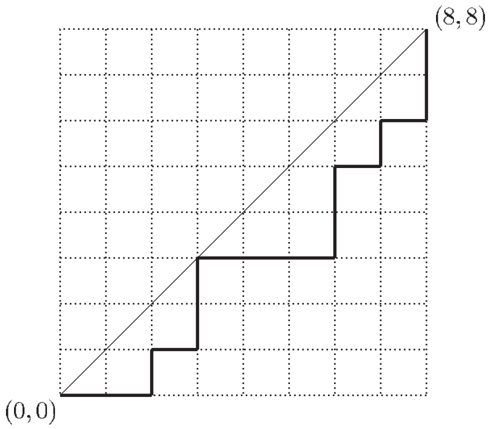

Figure 2. An example of a Dyck path of length 16. Dashed lines indicate grid lines of $\mathbb{Z}^2$. All the Dyck paths lie below the diagonal line.

where '$\Rightarrow$' denotes convergence in distribution, and $N(\mu, \sigma^2)$ denotes the Gaussian distribution with mean μ and variance σ^2. Equation (3) is equivalently expressed as

$$P_n\left(\sqrt{n}\left(\frac{S_{2,n}}{n} - \frac{1}{4}\right) \leqslant x\right) \to \frac{4}{\sqrt{2\pi}}\int_{-\infty}^{x} \mathrm{e}^{-8t^2}\mathrm{d}t \qquad \text{as} \quad n \to \infty.$$

In the same way as equation (2), we expect the following relations:

$$E\left(\frac{S_{r,n}}{S_{r-1,n}}\right) \to \frac{1}{4}, \quad E\left(\frac{S_{r,n}}{n}\right) \to \frac{1}{4^{r-1}} \qquad \text{as} \quad n \to \infty.$$

And, equation (3) is considered to be naturally generalized to

$$\sqrt{n}\left(\frac{S_{r,n}}{S_{r-1,n}} - \frac{1}{4}\right) \quad \Rightarrow \quad N\big(0, \sigma_r^2\big), \tag{4a}$$

$$\sqrt{n}\left(\frac{S_{r,n}}{n} - \frac{1}{4^{r-1}}\right) \quad \Rightarrow \quad N\big(0, \tilde{\sigma}_r^2\big), \tag{4b}$$

where σ_r^2 and $\tilde{\sigma}_r^2$ are variances depending on the order r. However, the proof of equations (4) has not been performed analytically or numerically so far, and the values of σ_r and $\tilde{\sigma}_r$ have not been obtained for $r \geqslant 3$. In the present paper, we propose a method for the numerical generation of random binary trees, using a kind of binary sequence referred to as a 'Dyck sequence'. Moreover, the random variable $S_{r,n}(T)$ can be calculated from the corresponding Dyck sequence of a binary tree T. Furthermore, we show numerically the validity of equations (4) and determine the values of σ_r and $\tilde{\sigma}_r$.

2. Correspondence between binary trees and Dyck paths

A *Dyck path* of length $2(n-1)$ is a sequence of points $(s_0, \ldots, s_{2(n-1)})$ on a two-dimensional lattice $\mathbb{Z}^2$ from $s_0 = (0, 0)$ to $s_{2(n-1)} = (n-1, n-1)$ such that each point $s_i = (x_i, y_i)$ satisfies $x_i \geqslant y_i$ and each elementary step (s_i, s_{i+1}) is either rightward or upward (see figure 2).

For each Dyck path, a binary sequence of length $2(n-1)$ is generated by replacing a rightward step with '1' and an upward step with '0'. The binary sequences generated by this

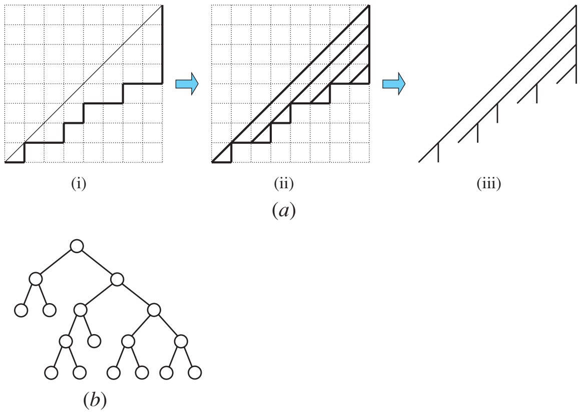

Figure 3. (*a*) An illustration of how to get a binary tree from a Dyck path. (i) The initial Dyck path of length 16. (ii) The Dyck path with diagonals from upper right to lower left. (iii) The diagonals and vertical steps. The structure of a binary tree can be seen. (*b*) The binary tree corresponding to (*a*-iii).

replacement are formally called *Dyck words on the alphabet* $\{1, 0\}$ [25], and for simplicity we call them *Dyck sequences* throughout the paper. Clearly, Dyck sequences share two properties: (i) the total number of '0' (and also '1') is $n - 1$, (ii) cumulative number of '0' is never greater than that of '1'.

A correspondence between the Dyck paths of length $2(n - 1)$ and the binary trees of magnitude n is explained as follows (see figure 3 for reference). (i) Start with a Dyck path of length $2(n - 1)$. (ii) Draw diagonal lines from upper right to lower left which are never below the Dyck path. (iii) Extract only the diagonals and the vertical lines from the Dyck path. It is found that the pattern obtained from this process is topologically the same as a binary tree of magnitude n, shown in figure 3(*b*). Note that each Dyck path has a one-to-one correspondence to a binary tree. Therefore, a Dyck path possesses the same topological structure as the corresponding binary tree.

The above method generates a binary tree from a Dyck sequence. Inversely, we can formulate a method for generating a Dyck sequence from a binary tree. Here, a binary tree is regarded as a graph representing a successive merging process of two adjacent nodes, and each merging is expressed by putting two nodes in parentheses '( )'. Thus, the topological structure of a binary tree $T \in \Omega_n$ is fully expressed by a sequence of the leaves $v_1, \ldots, v_n$ of T and $n - 1$ pairs of '( )' (an example is shown as step (i) in figure 4). A correspondence from a binary tree $T \in \Omega_n$ to a Dyck sequence of length $2(n - 1)$ consists of the following two steps. (i) Convert T into a sequence of $v_1, \ldots, v_n$ and '( )'. (ii) Eliminate 'v_1' and '(', and replace $v_2, \ldots, v_n$ with '1' and ')' with '0'. A generated binary sequence proves to be a Dyck sequence and the correspondence is one-to-one. Figure 4 illustrates this correspondence. Note that this process is similar to an expression tree and reverse Polish notation in formula manipulation [26].

The Horton–Strahler indices of a binary tree can be calculated through the corresponding Dyck sequence. The method consists of the following two steps. (i) Add '1' to the top of the Dyck sequence. (ii) Replace a segment '$m\ n\ 0$' ($m, n > 0$) with a single number '$\max\{m, n\} + \delta_{m,n}$' recursively until the length of a sequence becomes 1. For $r \geqslant 2$, we can obtain $S_{r,n}(T)$ by counting the number of the segment '$(r - 1)\,(r - 1)\,0$'. Note that operation (ii) is similar to equation (1) as shown in figure 5.

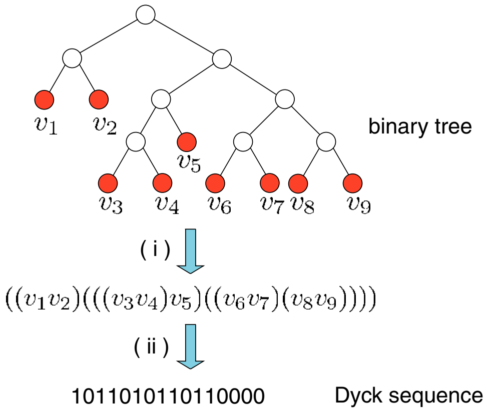

Figure 4. An illustration of the correspondence between a binary tree of magnitude 9 and a Dyck sequence of length 16. In step (i), a binary tree is converted into a sequence consisting of $v_1, \ldots, v_9$ and '( )'. In step (ii), a Dyck sequence is generated by the rule of replacement.

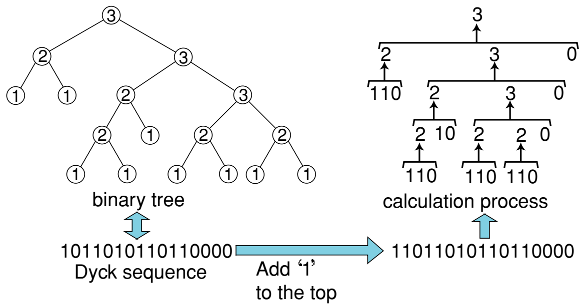

Figure 5. Similarity between a structure of the Horton–Strahler indices and the corresponding calculation process.

3. Generation of random Dyck paths

A basic method for the generation of random Dyck paths is summarized in [27]. In this section, we present a method in a little different manner from [27]. We also propose a graphical representation for the generation process.

Let $\mathcal{D}$ denote the set of points in $\mathbb{Z}^2$ where at least one Dyck path passes, that is, $\mathcal{D} \equiv \{(x, y) \in \mathbb{Z}^2 \mid 0 \leqslant x, y \leqslant n-1,\ x \geqslant y\}$. We assign 'transition probabilities' $P_\rightarrow(x, y)$ and $P_\uparrow(x, y)$ on each point $(x, y) \in \mathcal{D}$. Each elementary step (s_i, s_{i+1}) of a Dyck path $(s_1, \ldots, s_{2(n-1)})$ is selected stochastically: stepping rightward with a probability $P_\rightarrow(s_i)$ and upward with $P_\uparrow(s_i)$. A set of transition probabilities $\{P_\rightarrow(s), P_\uparrow(s) \mid s \in \mathcal{D}\}$ yields the generation probability of a Dyck path $(s_0, \ldots, s_{2(n-1)})$, which is given by

$$P(s_0, \ldots, s_{2(n-1)}) = \prod_{i=0}^{2(n-1)-1} p_i, \quad \text{where} \quad p_i = \begin{cases} P_\rightarrow(s_i), & \text{if } (s_i, s_{i+1}) \text{ is rightward,} \\ P_\uparrow(s_i), & \text{if } (s_i, s_{i+1}) \text{ is upward.} \end{cases}$$

Since we focus on the random binary-tree model, we need to determine the transition probabilities where every Dyck path is generated equiprobably.

We define a *monotonic path* from $(x, y) \in \mathcal{D}$ as a sequence of points on $\mathcal{D}$ from (x, y) to $(n-1, n-1)$ where each elementary step is either rightward or upward. Clearly, the length of a monotonic path from (x, y) is $2(n-1)-(x+y)$, and a monotonic path from $(0, 0)$ is identical to a Dyck path. The total number $\mathcal{N}(x, y)$ of the monotonic paths from (x, y) is written as

$$\begin{aligned}\mathcal{N}(x, y) &= \binom{2(n-1)-(x+y)}{n-x-1} - \binom{2(n-1)-(x+y)}{n-x-2} \\ &= \frac{\{2(n-1)-(x+y)\}!}{(n-1-x)!(n-y)!}(x-y+1).\end{aligned} \tag{5}$$

For the calculation of equation (5), we employed the reflection principle familiar in random-walk theory [28].

There are several remarks on $\mathcal{N}(x, y)$.

(1) For any $(x, y) \in \mathcal{D}$, $\mathcal{N}(x, y)$ is positive.
(2) $\mathcal{N}(n-1, y) = 1$, when $y = 0, \ldots, n-1$.
(3) If (x, y) is on the diagonal (i.e. $(x, y) = (k, k)$), then $\mathcal{N}(k, k) = \frac{\{2(n-k-1)\}!}{(n-1-k)!(n-k)!}$, which is known as the $(n-k-1)$st Catalan number [29].
(4) The number of Dyck paths (which can be expressed as $\mathcal{N}(0, 0)$) is given by the $(n-1)$st Catalan number. This is a well-known result, going back to Cayley [30].
(5) $\mathcal{N}(x, y) = \mathcal{N}(x+1, y) + \mathcal{N}(x, y+1)$ for all $(x, y) \in \mathcal{D}$, where we set $\mathcal{N}(x, y) = 0$ if $(x, y) \notin \mathcal{D}$.

At each point $(x, y) \in \mathcal{D}$, we define the transition probabilities $P_{\rightarrow}(x, y)$ and $P_{\uparrow}(x, y)$ as

$$P_{\rightarrow}(x, y) = \frac{\mathcal{N}(x+1, y)}{\mathcal{N}(x, y)} = \frac{(n-1-x)(x-y+2)}{(1+x-y)\{2(n-1)-(x+y)\}}, \tag{6a}$$

$$P_{\uparrow}(x, y) = \frac{\mathcal{N}(x, y+1)}{\mathcal{N}(x, y)} = \frac{(n-y)(x-y)}{(1+x-y)\{2(n-1)-(x+y)\}}. \tag{6b}$$

Specifically, $P_{\rightarrow} + P_{\uparrow} \equiv 1$, $P_{\uparrow}(k, k) = 0$ and $P_{\rightarrow}(n-1, y) = 0$. It is also proved inductively that equations (6) realize random generation of Dyck paths.

Next, we propose a graphical representation of random Dyck paths. The number $\mathcal{N}(x, y)$ can be calculated graphically as follows.

(1) Set $\mathcal{N}(n-1, y) = 1$ for all the rightmost points $(n-1, y)$ $(y = 0, \ldots, n-1)$ of $\mathcal{D}$. This implies that there is only one monotonic path from $(n-1, y)$, which is composed only of upward steps.
(2) For convenience, let $\mathcal{N}(x, y) = 0$ for all $(x, y) \notin \mathcal{D}$.
(3) $\mathcal{N}(x, y)$ is calculated from $\mathcal{N}(x, y) = \mathcal{N}(x+1, y) + \mathcal{N}(x, y+1)$, that is, $\mathcal{N}(x, y)$ is given by the sum of the value N on the right and upper adjacent points; thus, $\mathcal{N}(x, y)$ is determined from right to left, top to bottom. This implies that the monotonic paths from (x, y) consist of the ones passing through $(x+1, y)$ and $(x, y+1)$.

Note that $\mathcal{N}(x, y)$ determined from (i)–(iii) is identical to equation (5). The graphical representation and examples of generation probability are depicted in figure 6. We can roughly confirm the uniformity of generated Dyck paths through successive canceling.

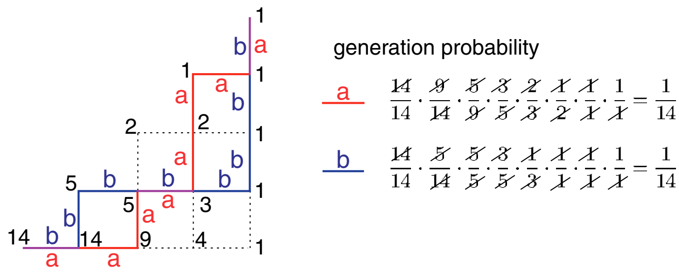

Figure 6. An example of the graphical representation of generation probability ($n = 5$). The dashed lines indicate the grid line of $\mathcal{D}$. Each number near a lattice point indicates $\mathcal{N}(x, y)$. From successive canceling, we can see that two paths (a and b) are generated with the same probability.

4. Numerical procedure

The cumulative distribution function of $N(0, \sigma^2)$ is given by

$$\int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}\sigma} \mathrm{e}^{-\frac{t^2}{2\sigma^2}} \, \mathrm{d}t = \frac{1}{2} \operatorname{erf}\left(\frac{x}{\sqrt{2}\sigma}\right) + \frac{1}{2}, \tag{7}$$

where $\operatorname{erf}(x)$ is the error function defined as

$$\operatorname{erf}(x) \equiv \frac{2}{\sqrt{\pi}} \int_0^x \mathrm{e}^{-t^2} \mathrm{d}t.$$

Thus, the central limit theorems (4*a*) and (4*b*) are respectively rewritten as

$$P_n\left(\sqrt{n}\left(\frac{S_{r,n}}{S_{r-1,n}} - \frac{1}{4}\right) \leqslant x\right) \xrightarrow{n\to\infty} \frac{1}{2} \operatorname{erf}\left(\frac{x}{\sqrt{2}\sigma_r}\right) + \frac{1}{2}, \tag{8a}$$

$$P_n\left(\sqrt{n}\left(\frac{S_{r,n}}{n} - \frac{1}{4^{r-1}}\right) \leqslant x\right) \xrightarrow{n\to\infty} \frac{1}{2} \operatorname{erf}\left(\frac{x}{\sqrt{2}\tilde{\sigma}_r}\right) + \frac{1}{2}. \tag{8b}$$

A numerical algorithm for the calculation of σ_r and $\tilde{\sigma}_r$ is summarized as follows.

(1) Generate Dyck sequences of length $2(n - 1)$ randomly, on the basis of the method in section 3.
(2) Calculate Horton–Strahler indices of the Dyck sequences.
(3) Compute values of both $\sqrt{n}\big(\frac{S_{r,n}}{S_{r-1,n}} - \frac{1}{4}\big)$ and $\sqrt{n}\big(\frac{S_{r,n}}{n} - \frac{1}{4^{r-1}}\big)$ for $r = 2, 3, \ldots$.
(4) Make cumulative distributions from the values, and then determine the values of σ_r and $\tilde{\sigma}_r$ by fitting equation (7) to the distribution functions.

5. Results of the central limit theorem

Figure 7 shows cumulative distributions of $\sqrt{n}\big(\frac{S_{r,n}}{S_{r-1,n}} - \frac{1}{4}\big)$ and $\sqrt{n}\big(\frac{S_{r,n}}{n} - \frac{1}{4^{r-1}}\big)$ generated from 10^5 samples with $n = 10\,000$. The stepwise increases appear in the cases of $r = 6$ and 7 in figure 7(*a*), because the denominator $S_{r-1,n}$ of a fraction $\frac{S_{r,n}}{S_{r-1,n}}$ is decreasing with respect to r.

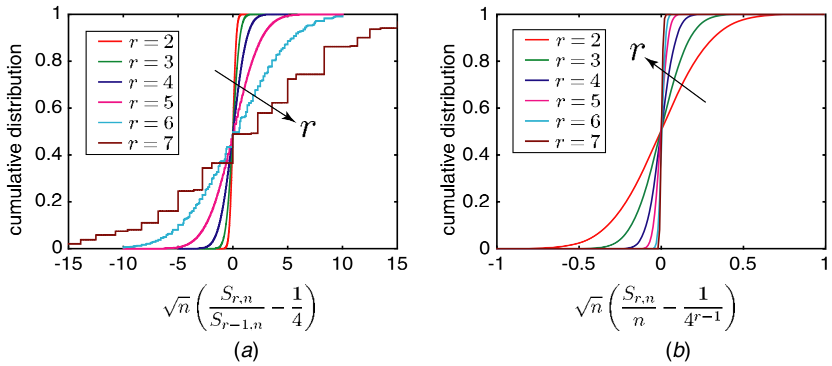

Figure 7. The cumulative distributions of (*a*) $\sqrt{n}(\frac{S_{r,n}}{S_{r-1,n}} - \frac{1}{4})$, and (*b*) $\sqrt{n}(\frac{S_{r,n}}{n} - \frac{1}{4^{r-1}})$ with $n = 10\,000$, $r = 2$–7, generated from 10^5 samples. Variance is increasing with respect to r in (*a*), and decreasing in (*b*) (indicated by the directions of the arrows).

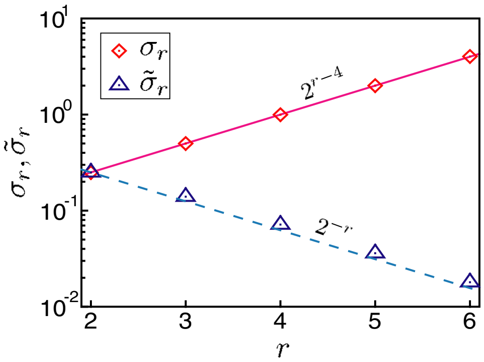

Figure 8. r-dependence of σ_r and $\tilde{\sigma}_r$. The solid and dashed lines indicate the functions 2^{r-4} and 2^{-r}, respectively.

Table 1. Values of σ_r and $\tilde{\sigma}_r$ obtained by fitting.

r	σ_r	2^{r-4}	$\tilde{\sigma}_r$	2^{-r}	$-\log_2 \tilde{\sigma}_r$
2	0.2492 ± 0.0001	0.25	0.2502 ± 0.0004	0.25	2.00
3	0.5000 ± 0.0001	0.5	0.1397 ± 0.0003	0.125	2.84
4	0.9967 ± 0.0004	1	0.0716 ± 0.0001	0.0625	3.80
5	2.0085 ± 0.0003	2	0.0361 ± 0.0004	0.031 25	4.79
6	4.025 ± 0.002	4	0.0181 ± 0.0009	0.015 625	5.79

By fitting of the distribution function (7) to each data set in figure 7, we obtain table 1 and figure 8, which suggest the relations

$$\sigma_r = 2^{r-4}, \tag{9a}$$

$$\tilde{\sigma}_r = \frac{1}{2^r}. \tag{9b}$$

Equation (9*a*) is in good agreement with our numerical results. Equation (9*b*) also seems to be consistent with our results, although there are errors of about a few per cent ($\leqslant$4%) between r and $-\log_2 \tilde{\sigma}_r$.

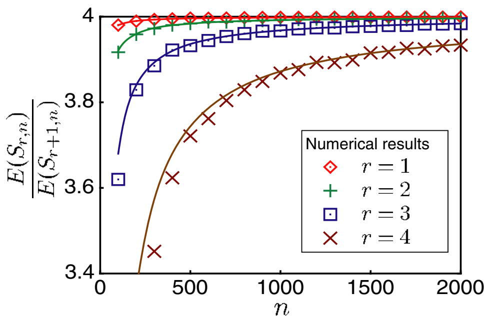

Figure 9. Comparison between analytical and numerical results of bifurcation ratios. Points denote the numerical result, and lines denote asymptotic forms $4 - \frac{4^r}{2n}$ for $r = 1, 2, 3, 4$. Numerical data are generated from 10^5 samples for each n at intervals of 100.

In conclusion, the two central limit theorems are stated as

$$\sqrt{n}\left(\frac{S_{r,n}}{S_{r-1,n}} - \frac{1}{4}\right) \quad \Rightarrow \quad N(0, 4^{r-4}), \tag{10a}$$

$$\sqrt{n}\left(\frac{S_{r,n}}{n} - \frac{1}{4^{r-1}}\right) \quad \Rightarrow \quad N(0, 4^{-r}). \tag{10b}$$

Note that both equations (10) are reduced to equation (3) when $r = 2$.

6. Discussion

With the presented method, we can directly calculate the Horton–Strahler indices from a Dyck sequence, without a binary tree. This effectiveness is caused by the translation between a binary tree and a Dyck sequence. The Horton–Strahler index is based on 'merging' or 'joining' of branches in a binary tree, and a Dyck sequence generated from the method in section 2 preserves a merging structure of the initial binary tree. Thus, the correspondence presented in this paper is suitable for the calculation of Horton–Strahler indices, and the similarity of the calculation process (figure 5) is obtained. It is known that there are some other ways for a one-to-one correspondence between Dyck paths and binary trees [29, 31, 32]. However, Dyck paths generated from such other methods are not directly connected to the Horton–Strahler indices.

Our method is quite universal for numerical calculations of the random binary-tree model, and various numerical calculations can be done other than the central limit theorems. For example, as shown in figure 9, our method is able to reproduce an asymptotic expansion of the bifurcation ratio

$$\frac{E(S_{r,n})}{E(S_{r+1,n})} = 4 - \frac{4^r}{2n} + O(n^{-2}) \quad r \geqslant 1 \tag{11}$$

quite well, which has been obtained analytically by Moon [33].

The central limit theorem is an essential tool for statistical characterization of branching patterns, but the generality of the central limit theorem is not obvious for actual branching systems. We believe that the central limit theorem for the bifurcation ratio is robust for some actual systems, and a lot of case studies are needed for checking the generality.

Generation of random Dyck paths can be regarded as a Markov process on $\mathcal{D}$, which is called the Bernoulli excursion [34]. In addition, by taking a certain scaling limit, the Bernoulli excursion converges weakly to a diffusion process called the Brownian excursion [35], which is defined as one-dimensional Brownian motion $\{B(t) : 0 \leqslant t \leqslant 1\}$ such that $P(B(0) = 0) = P(B(1) = 0) = 1$ and $P(B(t) \geqslant 0) = 1$ for $0 \leqslant t \leqslant 1$. We expect that some asymptotic properties of the random binary-tree model are derived from the corresponding scaling limit.

Furthermore, the number $\mathcal{N}(x, y)$ given by equation (5) is an example of the Kostka number, appearing in some combinatorial problems [36, 37]. It is expected that such other systems are related to a generation of random Dyck paths.

7. Conclusion

In the present paper, we propose a basic method for the numerical calculation of the random binary-tree model. Instead of a binary tree, Dyck sequences are generated randomly by using the transition probabilities (6). The scheme of branch ordering is also inherited to the Dyck-sequence representation. From numerical results, we confirm that the variances σ_r and $\tilde{\sigma}_r$ are determined as equations (9). Therefore, the validity of the central limit theorems (10) is suggested numerically.

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