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Topological Self-similarity on the Random Binary-Tree Model

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Abstract Asymptotic analysis on some statistical properties of the random binary-tree model is developed. We quantify a hierarchical structure of branching patterns based on the Horton-Strahler analysis. We introduce a transformation of a binary tree, and derive a recursive equation about branch orders. As an application of the analysis, topological self-similarity and its generalization is proved in an asymptotic sense. Also, some important examples are presented.

Keywords Branching pattern · Binary tree · Hierarchical structure · Horton-Strahler analysis · Topological self-similarity · Asymptotic behavior

1 Introduction

Branching patterns are universal in nature, including river networks, blood vessels, and dendritic crystals [1, 2]. They usually exhibit intricate forms (some patterns have been treated as fractal or multifractal objects). Branching structures are also fundamental and important tools for illustrating some data structures in computer science [3] and the classification of species in taxonomy [4]. Data structures and classification trees are simply graph-theoretic objects, and they have no geometrical structures such as length, angle and spatial symmetry. Instead of geometrical properties, topological (or graph-theoretic) properties are important for the analysis of such conceptual trees.

The topological structure of a branching pattern is expressed by a binary tree if the pattern is loopless and all the branching points are two-pronged. A binary tree can be regarded as a nested structure of the parent-child relations of nodes (see Fig. 1). In order to derive quantitative characteristics about binary trees, Horton [5] has introduced the idea of branch ordering. For mathematical convenience, Horton's method has been refined by Strahler [6]. The basic idea of their method is the assignment of numbers, referred to as the *Horton-Strahler index*, to the nodes of a binary tree.

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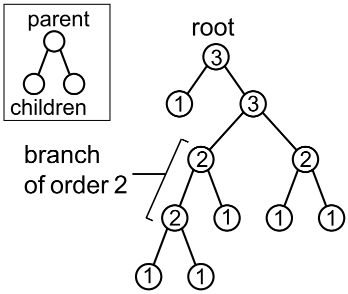


Fig. 1 A binary tree of magnitude 6. Nodes are represented by *open circles*, and the *numbers* on them are the corresponding Horton-Strahler indices

The Horton-Strahler ordering for a binary tree is defined recursively as follows (see also Fig. 1): (i) each leaf is assigned the order 1, (ii) a node whose children are both rth is assigned $r+1$, (iii) a node whose children are r_1th and r_2th ($r_1 \neq r_2$) is assigned $\max\{r_1, r_2\}$. In a binary tree, rth *branch* is defined as a maximal path connecting rth nodes. The ratio of the number of branches between two subsequent orders is called *bifurcation ratio*. It has been revealed that the bifurcation ratios become almost constant for different orders in some actual branching patterns [6–11], which is referred to as *topological self-similarity* [12, 13]. As a typical instance, many river networks possess their bifurcation ratios between 3 and 5 irrespective of orders [5, 12, 13]. The relevance of two types of self-similarity, 'original' self-similarity and topological self-similarity, has been considered in ramification analysis [14–19].

The number of leaves of a binary tree is called *magnitude*, and let Ω_n denote the set of topologically different binary trees of magnitude n. The number of the elements of Ω_n is given by

$$\sharp\Omega_n = \frac{(2n-2)!}{n!(n-1)!} \equiv c_{n-1}, \tag{1}$$

which is known as the $(n-1)$th Catalan number [20]. One of the simplest model of a branching structure is called the *random model* [21], where all the binary trees in Ω_n emerge randomly. More accurately, the random model is a probability space (Ω_n, P), where P represents the uniform probability measure on Ω_n, i.e., every binary tree $T \in \Omega_n$ has the same statistical weight $1/c_{n-1}$. We denote by $E_n[\cdot]$ an average over Ω_n. We introduce a random variable $S_{r,n} : \Omega_n \to \mathbb{N} \cup \{0\}$ such that $S_{r,n}(T)$ represents the number of rth branches in a binary tree $T \in \Omega_n$. Specifically, $S_{1,n}(T) \equiv n$ for all the binary tree $T \in \Omega_n$.

The rth bifurcation ratio $R_{r,n}$ on (Ω_n, P) is defined as

$$R_{r,n} = \frac{E_n[S_{r,n}]}{E_n[S_{r+1,n}]} \quad (r = 1, 2, \ldots),$$

and topological self-similarity has been confirmed in the case where magnitude n is sufficiently large. In fact, Moon [22] has derived

$$E_n[S_{r,n}] = 4^{1-r}n + \frac{1-4^{1-r}}{6} + O(n^{-1}),$$

and

$$R_{r,n} = 4 - \frac{4^r}{2n} + O(n^{-2}) \to 4 \quad (n \to \infty). \tag{2}$$

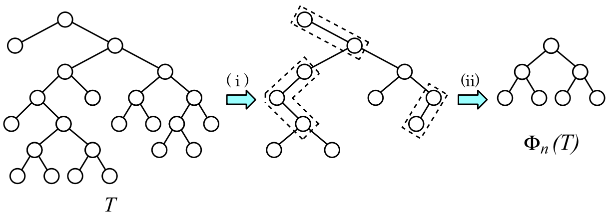


Fig. 2 An illustration of Φ_n for $n = 12$: (i) removal of the leaves of T, (ii) contraction

Therefore, the random model is topologically self-similar in an asymptotic sense, and the limit value of $R_{r,n}$ is 4. Moreover, the present authors [23] have derived

$$\frac{E_n[S^p_{r,n}]}{E_n[S^p_{r+1,n}]} = 4^p - \frac{4^{p+r-1}p^2}{2n} + O(n^{-2}) \to 4^p, \tag{3}$$

and this relation can be regarded as a generalization of (2). Other results on the Horton-Strahler analysis and tree structures are found in Refs. [24–33].

In the present paper, we focus on a random variable $f(S_{r,n})$, where $f : \mathbb{N} \cup \{0\} \to \mathbb{R}$ (or $\mathbb{C}$) is a certain function (further assumptions for f are stated in Sect. 3). We first derive a recursive relation between $E_n[f(S_{r,n})]$ and $E_m[f(S_{r-1,m})]$. Then, we also derive the asymptotic form of $E_n[f(S_{r,n})]$, and show topological self-similarity about f (or simply referred to as *generalized* topological self-similarity), in the sense that f-bifurcation ratio

$$R^f_{r,n} = \frac{E_n[f(S_{r,n})]}{E_n[f(S_{r+1,n})]}$$

is asymptotically independent of r. Clearly, $R^f_{r,n}$ is reduced to $R_{r,n}$ when $f(x) = x$.

2 Transformation of Binary Tree

First, we introduce a transformation Φ_n. For a binary tree $T \in \Omega_n$, a new binary tree $\Phi_n(T)$ is constructed from the following two steps: (i) remove all the leaves from T, (ii) if a node with only one child appears, such a node is merged with its child (this operation is called *contraction* in graph theory). Figure 2 illustrates these two steps. The magnitude of $\Phi_n(T)$ is at most $\lfloor n/2 \rfloor$, because a pair of first-order branches is needed to create a second-order branch. Hence,

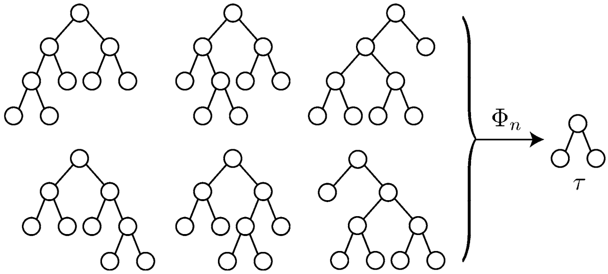
$$\Phi_n : \Omega_n \to \bigcup_{m=1}^{\lfloor \frac{n}{2} \rfloor} \Omega_m.$$

We introduce $\Omega^m_n = \Phi^{-1}_n(\Omega_m)$, which is explicitly expressed as $\Omega^m_n = \{T \in \Omega_n;\, S_{2,n}(T) = m\}$. Clearly, each binary tree $T \in \Omega_n$ belongs to some Ω^m_n, and this number m is uniquely determined as $m = S_{2,n}(T)$. Therefore, $\{\Omega^m_n\}_m$ is a partition of Ω_n (see Fig. 5(a) for reference), that is,

$$\Omega_n = \bigcup_{m=1}^{\lfloor \frac{n}{2} \rfloor} \Omega^m_n, \quad \Omega^m_n \cap \Omega^{m'}_n = \emptyset \ (m \neq m').$$

By definition, we have $S_{r-1,m}(\Phi_n(T)) = S_{r,n}(T)$ if $T \in \Omega^m_n$, and we regard that this is a relation which connects variables about two subsequent orders (rth and $(r-1)$th). For example, as for the binary tree T in Fig. 2 ($n = 12$, $m = 4$), we can easily check the following

Fig. 3 Some binary trees are mapped to the identical binary tree by Φ_n. The multiplicity in this case is $\mu_5^2(\tau) = 6$ ($n = 5$, $m = 2$)



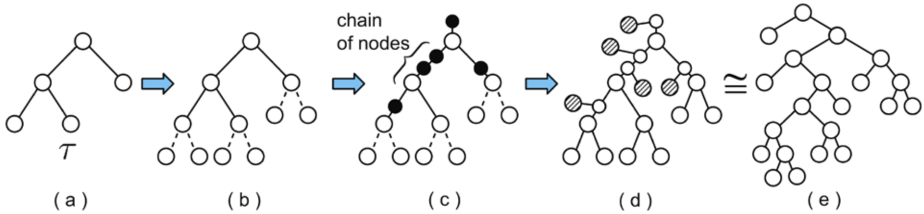


Fig. 4 An example of $\Phi_n^{-1}(\tau)$ for $n = 11$ and $m = 3$: (**a**) an initial binary tree $\tau \in \Omega_m$, (**b**) a pair of nodes is attached to each leaf of τ (indicated by the *dashed lines*), (**c**) intermediate nodes (*black nodes* in the figure) are added, (**d**) new leaves (*hatched nodes*) are attached to the intermediate nodes, and (**e**) generated binary tree

relations:

$$S_{1,m}(\Phi_n(T)) = 4 = S_{2,n}(T), \qquad S_{2,m}(\Phi_n(T)) = 2 = S_{3,n}(T),$$
$$S_{3,m}(\Phi_n(T)) = 1 = S_{4,n}(T).$$

Note that the restriction $\Phi_n|_{\Omega_n^m} : \Omega_n^m \to \Omega_m$ is not one-to-one. That is, some binary trees degenerate into the same binary tree by the action of Φ_n (see Fig. 3 for example). Then, for a binary tree $\tau \in \Omega_m$ $(1 \le m \le \lfloor n/2 \rfloor)$, we introduce the multiplicity of degeneracy

$$\mu_n^m(\tau) = \sharp\{T \in \Omega_n | \Phi_n(T) = \tau\} \equiv \sharp\Phi_n^{-1}(\tau).$$

In order to calculate $\mu_n^m(\tau)$, we trace the inverse process $\Phi_n^{-1}(\tau)$. As mentioned above, Φ_n is a removal of the leaves of a binary tree, and multiplicity μ_n^m is concerned with a contraction process. Thus, the inverse process $\Phi_n^{-1}(\tau)$ can be formed by attaching n leaves to τ in the following way.

(i) A pair of nodes is attached to each leaf of τ.
(ii) $n - 2m$ 'intermediate' nodes are added in the form of a chain, which is the inverse of contraction. The number of different ways of adding amounts to $\binom{n-2}{n-2m}$.
(iii) $n - 2m$ leaves are attached to the nodes added in (ii). Each leaf can be attached independently from either left or right, thus the total number of ways of choosing sides is given by 2^{n-2m}.

A series of procedures is presented in Fig. 4. From these steps, the total multiplicity $\mu_n^m(\tau)$ is calculated as

$$\mu_n^m(\tau) = \binom{n-2}{n-2m} 2^{n-2m}. \tag{4}$$

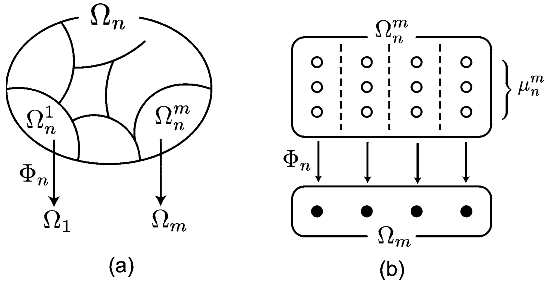


Fig. 5 A schematical illustration of Ω_n^m, Φ_n, and μ_n^m. (**a**) $\{\Omega_n^m\}_m$ is a partition of Ω_n, and $\Phi_n(\Omega_n^m) = \Omega_m$. (**b**) The *open* and *solid circles* represent individual binary trees (the elements of Ω_n^m and Ω_m, respectively). The elements in Ω_n^m can be arrayed rectangularly, where the vertically aligned elements in Ω_n^m are mapped to the identical binary tree in Ω_m

The calculation of (4) and the above process (i)–(iii) only involve n and m, and $\mu_n^m(\tau)$ is equal for each $\tau \in \Omega_m$. Therefore, we hereafter write $\mu_n^m \equiv \mu_n^m(\tau)$ with no confusion (in other words, $\Phi_n^{-1}(\tau) = \mu_n^m$ for all $\tau \in \Omega_m$). Since the transformation $\Phi_n : \Omega_n^m \to \Omega_m$ is surjective (onto), the elements of Ω_n^m can be aligned as in Fig. 5(b). The relation between Ω_n^m, Ω_m, and μ_n^m is expressed as

$$\mu_n^m = \frac{\sharp\Omega_n^m}{\sharp\Omega_m}. \tag{5}$$

By (1), (4), and (5), the number of the elements of Ω_n^m is expressed as

$$\sharp\Omega_n^m = \mu_n^m \cdot \sharp\Omega_m = \binom{n-2}{n-2m} 2^{n-2m} \frac{(2m-2)!}{m!(m-1)!} = \frac{(n-2)!\,2^{n-2m}}{(n-2m)!\,m!\,(m-1)!}.$$

Therefore, the average of random variable $f(S_{r,n})$ is expressed as

$$\begin{aligned}
E_n[f(S_{r,n})] &= \frac{1}{c_{n-1}} \sum_{T\in\Omega_n} f(S_{r,n})(T) \\
&= \frac{1}{c_{n-1}} \sum_{m=1}^{\lfloor \frac{n}{2} \rfloor} \sum_{T\in\Omega_n^m} f(S_{r,n})(T) \\
&= \frac{1}{c_{n-1}} \sum_{m=1}^{\lfloor \frac{n}{2} \rfloor} \sum_{T\in\Omega_n^m} f(S_{r-1,m})(\Phi_n(T)) \\
&= \frac{1}{c_{n-1}} \sum_{m=1}^{\lfloor \frac{n}{2} \rfloor} \mu_n^m \sum_{\tau\in\Omega_m} f(S_{r-1,m})(\tau) \\
&= \frac{1}{c_{n-1}} \sum_{m=1}^{\lfloor \frac{n}{2} \rfloor} \mu_n^m c_{m-1} E_m[f(S_{r-1,m})] \\
&= \frac{n!(n-1)!(n-2)!}{(2n-2)!} \sum_{m=1}^{\lfloor \frac{n}{2} \rfloor} \frac{2^{n-2m}}{(n-2m)!m!(m-1)!} E_m[f(S_{r-1,m})].
\end{aligned} \tag{6}$$

Equation (6) is a recursive relation about rth variable $f(S_{r,n})$ and $(r-1)$th variable $f(S_{r-1,m})$. The present authors [23] have derived a similar recursive equation for the pth moments $E_n[S_{r,n}^p]$ and $E_m[S_{r-1,m}^p]$. Compared with the former result, (6) is more general and derivation is much easier. Yekutieli and Mandelbrot [24] have derived that the value

$$\frac{n!(n-1)!(n-2)!2^{n-2m}}{(2n-2)!(n-2m)!m!(m-1)}$$

is the probability of finding a binary tree of magnitude n with m branches of order 2.

3 Asymptotic Expansion of $E_n[f(S_{r,n})]$

In this section, we derive the asymptotic form of $E_n[f(S_{r,n})]$ by using the recursive equation (6). First, $f(S_{1,n}(T)) = f(n)$ is a constant on Ω_n because of the property $S_{1,n}(T) \equiv n$ $(T \in \Omega_n)$. Thus, we note the formula $E_n[f(S_{1,n})] = E_n[f(n)] = f(n)$. Let us assume that the function f has the following expansion:

$$E_n[f(S_{1,n})] \equiv f(n) = a_1 n^k + b_1 n^{k-1} + O(n^{k-2}). \tag{7}$$

Throughout this paper, we consistently use the symbols a and b to signify the coefficients of first and second leading terms respectively, and k to signify the leading order of the expansion. Equation (7) is the Laurent expansion of f around infinity. This type of expansion is valid if f does not have an essential singularity at infinity. Polynomial and rational functions are typical examples of such functions, and as we see in the following section, important random variables in the Horton-Strahler analysis are mostly polynomial or rational functions of $S_{r,n}$. Hence, even if (7) is supposed, a sufficient large class of important random variables on Ω_n is within the scope of the analysis.

We regard (7) as the initial condition of the recursive equation (6). We also assume that $E_n[f(S_{r,n})]$ has the form

$$E_n[f(S_{r,n})] = a_r n^k + b_r n^{k-1} + O(n^{k-2}), \tag{8}$$

where the coefficients a_r and b_r are independent of n.

According to Ref. [23], the asymptotic form of the pth moment of $S_{2,n}$ is expressed as

$$E_n[S_{2,n}^p] = \frac{1}{c_{n-1}} \sum_{m=1}^{\lfloor \frac{n}{2} \rfloor} \mu_n^m c_{m-1} m^p = \left(\frac{n}{4}\right)^p \left(1 + \frac{p^2}{2n}\right) + O(n^{p-2}). \tag{9}$$

By substituting (8) into (6) and using (9), the average of $f(S_{r,n})$ can be calculated as

$$\begin{aligned} E_n[f(S_{r,n})] &= \frac{1}{c_{n-1}} \sum_{m=1}^{\lfloor \frac{n}{2} \rfloor} \mu_n^m c_{m-1} \left(a_{r-1} m^k + b_{r-1} m^{k-1} + O(m^{k-2})\right) \\ &= a_{r-1} E_n\left[S_{2,n}^k\right] + b_{r-1} E_n\left[S_{2,n}^{k-1}\right] + O(n^{k-2}) \\ &= a_{r-1} \left(\frac{n}{4}\right)^k \left(1 + \frac{k^2}{2n}\right) + b_{r-1} \left(\frac{n}{4}\right)^{k-1} + O(n^{k-2}) \\ &= \frac{a_{r-1}}{4^k} n^k + \left(\frac{b_{r-1}}{4^{k-1}} + \frac{k^2 a_{r-1}}{2 \cdot 4^k}\right) n^{k-1} + O(n^{k-2}). \end{aligned} \tag{10}$$

Comparing $O(n^k)$ terms of (8) and (10), we get a recursive equation about $\{a_r\}_{r\in\mathbb{N}}$:

$$a_r = \frac{a_{r-1}}{4^k},$$

and the general solution a_r is

$$a_r = \left(\frac{1}{4^k}\right)^{r-1} a_1. \tag{11}$$

Similarly, $O(n^{k-1})$ terms yield an equation about $\{b_r\}_r$:

$$b_r = \frac{b_{r-1}}{4^{k-1}} + \frac{k^2 a_{r-1}}{2\cdot 4^k} = \frac{b_{r-1}}{4^{k-1}} + \frac{k^2 a_1}{2}\frac{1}{4^{kr}}.$$

The general solution of this equation is given by

$$b_r = \left(\frac{1}{4^{k-1}}\right)^{r-1} b_1 + \frac{k^2 a_1}{4^k}\frac{4^{r-1}-1}{6}. \tag{12}$$

Substituting (11) and (12) into (10), one can obtain

$$E_n[f(S_{r,n})] = \left(\frac{n}{4^{r-1}}\right)^k \left\{a_1 + \frac{1}{n}\left(4^{r-1}b_1 + \frac{4^{r-1}-1}{6}k^2 a_1\right)\right\} + O(n^{k-2}). \tag{13}$$

Equation (13) is the asymptotic expansion of $E_n[f(S_{r,n})]$.

A similar formula can be derived for a multi-variable function such as $f(S_{1,n}, S_{2,n})$ (two-variable), $f(S_{1,n}, S_{2,n}, S_{3,n})$ (three-variable) and so on. For example, assuming that a two-variable function f has the following expansion

$$E_n\big[f(S_{1,n}, S_{2,n})\big] = a_1 n^k + b_1 n^{k-1} + O(n^{k-2}), \tag{14}$$

then the asymptotic form of $E_n[f(S_{r,n}, S_{r+1,n})]$ is expressed as

$$E_n\big[f(S_{r,n}, S_{r+1,n})\big] = \left(\frac{n}{4^{r-1}}\right)^k \left\{a_1 + \frac{1}{n}\left(4^{r-1}b_1 + \frac{4^{r-1}-1}{6}k^2 a_1\right)\right\} + O(n^{k-2}). \tag{15}$$

4 Generalized Topological Self-similarity

Using the asymptotic expansions (13) or (15), we can easily show generalized topological self-similarity. The asymptotic formula of a generalized bifurcation ratio $R^f_{r,n}$ is calculated as

$$R^f_{r,n} \equiv \frac{E_n[f(S_{r,n})]}{E_n[f(S_{r+1,n})]} = 4^k - \frac{4^{k+r-1}(6b_1 + a_1 k^2)}{2a_1 n} + O(n^{-2}) \to 4^k \quad \text{as } n \to \infty. \tag{16}$$

Therefore, on the random binary-tree model, topological self-similarity about f is concluded in an asymptotic sense, if f has an expansion as in (7) or (14). Note that the first and second leading terms in (16) consists of a_1, b_1 and k, which are given in (7) as the initial condition. We also note that the limit value of $R^f_{r,n}$ depends only on the dominant order k of f.

Here, we provide three examples.

1. We start from $f(n)=n^k$ ($a_1=1$, $b_1=0$), and $E_n[f(S_{r,n})]=E_n[S_{r,n}^k]$ is the kth moment of $S_{r,n}$. In this case, (13) is reduced to

$$E_n[S_{r,n}^k]=\left(\frac{n}{4^{r-1}}\right)^k\left(1+\frac{4^{r-1}-1}{6n}k^2\right)+O(n^{k-2}),$$

and the asymptotic form of $R_{r,n}^f$ is

$$R_{r,n}^f=4^k-\frac{4^{k+r-1}k^2}{2n}+O(n^{-2}).$$

Thus, (3) is rederived from the formula (16).
2. We next consider the asymptotic property of the variance of $S_{r,n}$. By the definition $S_{1,n}\equiv n$, $\mathrm{var}(S_{1,n})=0$ is easily obtained. The analytical expression of the variance of $S_{2,n}$ is given by

$$\mathrm{var}(S_{2,n})\equiv E_n\big[(S_{2,n}-E_n[S_{2,n}])^2\big]=\frac{n(n-1)(n-2)(n-3)}{2(2n-3)^2(2n-5)}=\frac{n}{16}-\frac{1}{32}+O(n^{-1}), \tag{17}$$

which has been obtained by Werner [25]. We think that $\mathrm{var}(S_{1,n})=0$ is exceptional. Regarding (17) as the initial condition of calculation ($a_1=\frac{1}{16}$, $b_1=-\frac{1}{32}$, and $k=1$), the asymptotic form of $\mathrm{var}(S_{r,n})$ is calculated as

$$\mathrm{var}(S_{r,n})=\frac{n}{4^r}-\frac{1}{48}-\frac{1}{6\cdot 4^r}+O(n^{-1}).$$

Therefore, for sufficiently large n, the variance $\mathrm{var}(S_{r,n})$ decreases almost exponentially with an increase of r.
3. We next deal with a two-variable function $f(S_{1,n},S_{2,n})=S_{2,n}/S_{1,n}(=S_{2,n}/n)$. According to the result

$$E_n[S_{2,n}]=\frac{n(n-1)}{2(2n-3)}$$

obtained by Werner [25], the initial condition (14) in this case is calculated as

$$E_n\left[\frac{S_{2,n}}{S_{1,n}}\right]=E_n\left[\frac{S_{2,n}}{n}\right]=\frac{E_n[S_{2,n}]}{n}=\frac{n-1}{2(2n-3)}=\frac{1}{4}+\frac{1}{8n}+O(n^{-2}).$$

Thus, we have $a_1=\frac{1}{4}$, $b_1=\frac{1}{8}$ and $k=0$, and (15) yields

$$E_n\left[\frac{S_{r+1,n}}{S_{r,n}}\right]=\frac{1}{4}+\frac{4^{r-2}}{2n}+O(n^{-2}). \tag{18}$$

On the other hand, by using (2),

$$\frac{E_n[S_{r+1,n}]}{E_n[S_{r,n}]}=\frac{1}{R_{r,n}}=\frac{1}{4}+\frac{4^{r-2}}{2n}+O(n^{-2}). \tag{19}$$

In conclusion, from (18) and (19), we obtain

$$E_n\left[\frac{S_{r+1,n}}{S_{r,n}}\right]=\frac{E_n[S_{r+1,n}]}{E_n[S_{r,n}]}+O(n^{-2}). \tag{20}$$

$O(n^{-2})$ terms in the right hand side of (20) vanish only if $r = 1$, but when n is sufficiently large, these terms can neglect even $r \geq 2$.

5 Discussion

The random binary-tree model is highly simplified model, and its advantages are that analytical calculations can be widely performed, and that some of such calculations are valid for some actual patterns. Thus, the random model is important as a prototype of branching systems. In addition, another significance of the random model is concerned with statistical mechanics. A branching system with fluctuations can be regarded as a statistical ensemble, and each binary tree in Ω_n represents a microscopic state. From this point of view, the random model (Ω_n, P) is regarded as the microcanonical ensemble. (In fact, the uniform measure P corresponds to the principle of equal weight.) Therefore, the random model is helpful for the theoretical foundation of the statistical physics of branching systems.

We proved topological self-similarity about f on the random model, and we expect that such generalized topological self-similarity is also valid for some actual branching patterns. For example, topologically self-similar patterns, such as river networks, are expected to be topologically self-similar about f, for some class of f.

The random binary-tree model is a graph-theoretic model, where geometrical properties are all neglected. As a refinement of the Horton-Strahler analysis, ramification analysis [14–17] describes how many side-branches emerge. Ramification analysis is also a topological model, but it is connected with a fractal structure. Based on the methods and results in this paper, we expect that some asymptotic properties of random variables in ramification analysis are obtained, and that the more profound comprehension of a connection between topological self-similarity and original self-similarity can be obtained.

6 Conclusion

We have first introduced the transformation Φ_n in Sect. 2, and recursive equation (6) is derived. Equation (6) can be solved asymptotically, if $f(n)$ is expressed as in (7). Solution (13) is the asymptotic form of $E_n[f(S_{r,n})]$. A similar result (15) can be obtained for a two-variable function, and the generalization to multi-variable functions is straightforward. Topological self-similarity about f is confirmed in (16). We have also presented some examples of calculations.

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