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Optimizing the First-Passage Process on a Class of Fractal Scale-Free Trees

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Abstract: First-passage processes on fractals are of particular importance since fractals are ubiquitous in nature, and first-passage processes are fundamental dynamic processes that have wide applications. The global mean first-passage time (GMFPT), which is the expected time for a walker (or a particle) to first reach the given target site while the probability distribution for the position of target site is uniform, is a useful indicator for the transport efficiency of the whole network. The smaller the GMFPT, the faster the mass is transported on the network. In this work, we consider the first-passage process on a class of fractal scale-free trees (FSTs), aiming at speeding up the first-passage process on the FSTs. Firstly, we analyze the global mean first-passage time (GMFPT) for unbiased random walks on the FSTs. Then we introduce proper weight, dominated by a parameter w ($w > 0$), to each edge of the FSTs and construct a biased random walks strategy based on these weights. Next, we analytically evaluated the GMFPT for biased random walks on the FSTs. The exact results of the GMFPT for unbiased and biased random walks on the FSTs are both obtained. Finally, we view the GMFPT as a function of parameter w and find the point where the GMFPT achieves its minimum. The exact result is obtained and a way to optimize and speed up the first-passage process on the FSTs is presented.

Keywords: the global mean first-passage time; fractal scale-free trees; random walks on fractals



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1. Introduction

Many real-life networks, such as hyperlinks in the World Wide Web, protein–protein interaction networks and cellular networks [1–3], exhibit fractal and scale-free characters, and models for fractal scale-free networks have been a research hotspot [3–9]. The self-similar structures of these networks make it possible for us to analytically evaluate the topological and dynamic properties of these networks. Among a plethora of dynamic processes, the first-passage process is of particular important since many other dynamic processes can be analyzed and understood in terms of a first-passage process [10–12]. Typical examples include fluorescence quenching, where light emission stops when it reacts with a quencher; the stopping of the searching process for a wandering forager when it first reaches the target; and gene expression where the cell division event occurs when the copy number of the time-keeper protein hits a threshold for the first time [13,14]. An important quantity related to the first-passage process is the mean first-passage time (MFPT), referred to as $T_{i \rightarrow j}$, which is the expected time for a walker starting from site i to reach the target j for the first time. Averaging the MFPT over all the possible source and target sites, one can obtain the global mean first-passage time (GMFPT), referred to as $\langle GFPT \rangle$ and defined by

$$\langle GFPT \rangle = \frac{1}{N(N-1)} \sum_{j=1}^N \sum_{i \neq j} T_{i \rightarrow j}, \quad (1)$$

where N is the total number of nodes of the underlying networks.

In the past several decades, the first-passage properties have attracted lots of attention [15–18], and the mean first-passage time has been extensively studied. Some of them focus on disclosing the effects of the topology on the MFPT (or GMFPT), and lots of results have been obtained for unbiased random walks on different networks, such as Sierpinski gaskets [19,20], pseudofractal scale-free web [21,22], scale-free Koch networks [9,23], (u, v) flowers [24], and many fractal scale-free trees [9,21,25–27]. The MFPT and GMFPT are useful indicators for the transport efficiency of the network. These works uncovered the effects of the topology on the transport efficiency. There are also many works devoted to improving the transport efficiency by designing appropriate biased random walk strategies [28–30]. By introducing the proper weight to each edge of the network and designing a proper biased random walk strategy, one can shorten the MFPT to obtain higher transport efficiency on the underlying networks [31–35]. One can also shorten the GMFPT for random walks on some networks [36].

In this work, we extend the networks studied in Refs. [25,36] to a kind of general fractal scale-free trees, which are controlled by two integer parameters: u and v ($u \geq 1, v \geq 1$). The networks in the case $u = 1$ (or $u = 2$) are just the networks studied in Refs. [25,36]. Here, we study unbiased and biased random walks on the general fractal scale-free trees (FSTs), aiming at shortening the GMFPT and optimizing the transport efficiency of the networks. Firstly, we analyze the GMFPT for classical unbiased random walks on the FSTs. Then, we introduce the proper weight to each edge of the FSTs and design a proper biased random walk strategy, then evaluate the GMFPT analytically for biased random walks on the FSTs. Finally, we compare the results of the GMFPT for unbiased random walks and those for biased random walks and find the effects of the weights on the GMFPT. The way to shorten and minimize the GMFPT is found. Therefore, we obtain a way to optimize the first-passage process for random walks on the general fractal scale-free trees.

This paper is organized as follows. In Section 2, we describe the typologies of the fractal scale-free trees and the weighted fractal scale-free trees. Next, in Section 3, we evaluate the GMFPT for classical unbiased random walks on the FSTs. In Section 4, we analyze the GMFPT for biased random walks on the FSTs. In Section 5, we compare the GMFPT for unbiased random walks and the GMFPT for biased random walks on the FSTs and present the optimal parameters where the GMFPT achieves its minimum. Finally, conclusions and discussions are provided in Section 6, and detailed derivations are collected in the Appendixes.

2. Fractal Scale-Free Trees and the Weighted Fractal Scale-Free Trees

The networks considered here are deterministic networks that can be built in an iterative way. Let $G(n)$ denote the network of generation n ($n \geq 0$). The construction starts from two nodes connected by an edge, which corresponds to $G(0)$. For $n \geq 1$, $G(n)$ can be obtained from $G(n-1)$ in the following way. For each edge of $G(n-1)$, we replace it with a path of length u ($u \geq 1$) firstly, and then $2v$ new nodes are added; half of them are connected to one endpoint of the path and half of them are connected to another endpoint of the path. For convenience, we call the $2v$ new nodes with degree 1 as external nodes and the $u-1$ new nodes in the path with length u as internal nodes. In other words, $G(n)$ can be obtained from $G(n-1)$ by replacing each edge of $G(n-1)$ with the cluster on the right-hand side of Figure 1. The networks for the particular case $u = 1$ and $u = 2$ are just the networks studied in Refs. [25,36]. The construction process for the first three generations of the network in the particular case of $u = 3$, $v = 2$ are shown in Figure 2.

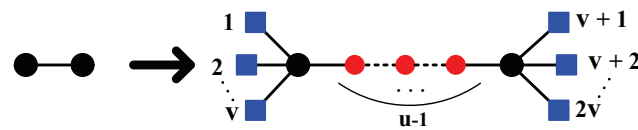


Figure 1. Iterative construction method of networks. $G(n)$ are obtained from $G(n-1)$ by replacing each edge of $G(n-1)$ with a cluster on the right-hand side of the arrow. The $2v$ blue nodes are called external nodes, and the $u-1$ red nodes are called internal nodes, while the two black nodes are the original two nodes of the path.

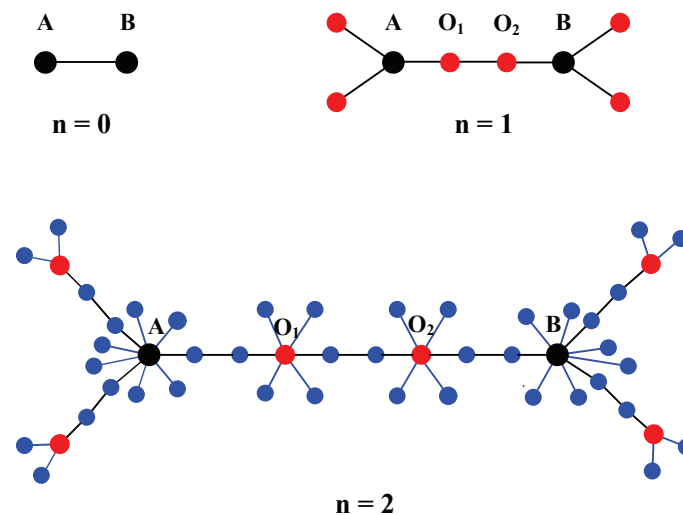


Figure 2. The first three generations of the particular network in the case of $u = 3, v = 2$. The black nodes are the hub nodes (the highest degree); the red circles are new nodes added at generation $n = 1$; the blue circles are new nodes added in generation $n = 2$.

According to the construction, we can easily know the total number of edges E_n of $G(n)$ is

$$E_n = (2v + u)^n, \quad (2)$$

and the total number of nodes N_n is

$$N_n = 1 + (2v + u)^n. \quad (3)$$

One can also find that, in the case $u = 1$, these kinds of networks are non-fractal, which means that they have infinite fractal dimension; and in the case of $u \geq 2$, they are fractals with the fractal dimension $d_f = \ln(2v + u) / \ln u$ [7]. Furthermore, they are scale-free trees with the distribution $P(k) \sim k^{-\gamma}$, where $\gamma = 1 + \frac{\ln(2v+u)}{\ln(v+1)}$ [7]. Therefore, in the case $u \geq 2$, we can call them fractal scale-free trees (FSTs).

Note that the first-passage properties for the networks with $u = 1$ and $u = 2$ were studied in Refs. [25,36]. In this paper, we just study the networks while $u \geq 2$. We study the tree-like networks because of their inherent interests and their correlation with real systems, where the so-called boundary tree is well known [37,38].

It is worth mentioning that the networks considered here have an equivalent construction method that highlights their self-similarity. As shown in Figure 3, the network with generation $n + 1$, referred to as $G(n + 1)$, is composed of $2v + u$ sub-units that are copies of $G(n)$, labeled by $G_k(n), k = 1, 2, \dots, 2v + u$, and connected to one another by their hubs (i.e., nodes with highest degree).

In order to construct the biased random walk strategy, we introduce weight to each edge of the fractal scale-free trees and obtain the weighted fractal scale-free trees in the following recursive way. For $n = 0$, the weight for the only edge of $G(0)$ is 1. For $n \geq 1$, it is known that $G(n)$ is obtained from $G(n-1)$ by replacing each edge of $G(n-1)$ with a

path of length u firstly, and then $2v$ new nodes are added; half of them are connected to one endpoint of the path and half of them are connected to another endpoint of the path. The weights for edges of $G(n)$ can be also obtained from the weights for edges of $G(n-1)$. The weights for the u new edges in the path with length u are the same as the weights for the original edge of $G(n-1)$, and the weights for the edges between the endpoints of the path and the $2v$ new nodes are set to be w ($w > 0$) times the weight of the original edge. Therefore, w is an important parameter that controls the weights for the edges of the networks. The weights for edges of the particular fractal scale-free trees in Figure 2 are shown in Figure 4.

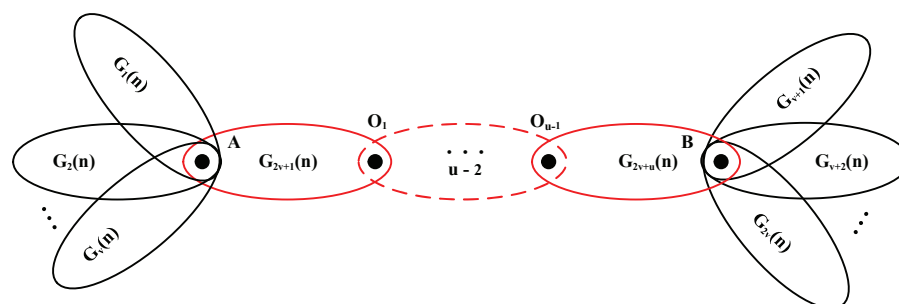


Figure 3. Alternative construction of the fractal scale-free trees, which highlights self-similarity. The network with generation $n+1$, denoted by $G(n+1)$, is composed of $2v+u$ sub-units, which are copies of $G(n)$, labeled as $G_1(n), G_2(n), \dots, G_{2v+u}(n)$, and connected to one another at their hubs.

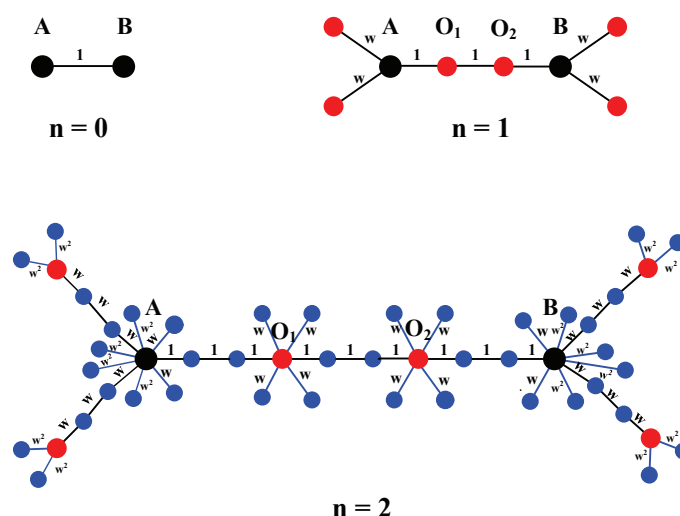


Figure 4. The weights for the edges of the particular fractal scale-free trees shown in Figure 2.

3. GMFPT for Unbiased Random Walk on the Fractal Scale-Free Trees

In this section, we analyze the GMFPT for classical unbiased random walks on fractal scale-free trees (FSTs). At any step, the walker at the current site i steps to any of its neighbors j with the same probability. This is to say, the transition probability from node i to node j can be written as

$$P_{ij} = \begin{cases} \frac{1}{d_i} & i \sim j \\ 0 & \text{otherwise} \end{cases}, \quad (4)$$

where d_i is the degree of node i , and $i \sim j$ means there is an edge between nodes i and j .

In order to show the evolution of the global mean first-passage time with the increase in the network size, here, $\langle GFPT \rangle_n$ represents $\langle GFPT \rangle$ for network $G(n)$. By exploring the connection between the MFPT and the effective resistance and the relation between the effective resistance and the shortest path length, the global mean first-passage time

(GMFPT), defined by Equation (1), for unbiased random walks on network $G(n)$ can be rewritten as [25]

$$\begin{aligned}\langle GFPT \rangle_n &= \frac{1}{N_n(N_n - 1)} \sum_{j=1}^{N_n} \sum_{i \neq j} T_{i \rightarrow j}(n) \\ &= \frac{2L_{sum}(n)}{N_n},\end{aligned}\quad (5)$$

where

$$L_{sum}(n) = \frac{1}{2} \sum_{j=1}^{N_n} \sum_{i \neq j} L_{ij}(n) \quad (6)$$

and $L_{ij}(n)$ denotes the shortest path length between nodes i to node j on network $G(n)$.

Note that $G(0)$ is just two nodes connected by an edge. It is easy to know $L_{sum}(0) = 1$. For $n \geq 0$, recalling the self-similar structure of fractal scale-free trees, as shown in Figure 4, the $G(n+1)$ is composed by $2v+u$ subunits, which are copies of $G(n)$, labeled by $G_k(n)$, $k = 1, 2, \dots, 2v+u$ and connected to one another by their hubs. We have

$$\begin{aligned}L_{sum}(n+1) &= \frac{1}{2} \sum_{i,j \in G(n+1), i \neq j} L_{ij} \\ &= \frac{1}{2} \sum_{k=1}^{2v+u} \sum_{i,j \in G_k(n), i \neq j} L_{ij} + \frac{1}{2} \sum_{k_1 \neq k_2} \sum_{i \in G_{k_1}(n)} \sum_{j \in G_{k_2}(n)} L_{ij} \\ &= (2v+u)L_{sum}(n) + \Delta_n,\end{aligned}\quad (7)$$

where $\Delta_n = \frac{1}{2} \sum_{k_1 \neq k_2} \sum_{i \in G_{k_1}(n)} \sum_{j \in G_{k_2}(n)} L_{ij}$ is the sum of shortest path between any two nodes that

belong to the different subunits of $G(n+1)$.

Using the Equation (7) recursively, for $n \geq 0$, we obtain

$$\begin{aligned}L_{sum}(n) &= (2v+u)L_{sum}(n-1) + \Delta_{n-1} \\ &= (2v+u)^2 L_{sum}(n-2) + (2v+u)\Delta_{n-2} + \Delta_{n-1} \\ &= \dots \\ &= (2v+u)^n L_{sum}(0) + \sum_{k=0}^{n-1} (2v+u)^{n-1-k} \Delta_k.\end{aligned}\quad (8)$$

For Δ_n , as derived in Appendix A,

$$\begin{aligned}\Delta_n &= (2v+u)^{2n+1}(2v+u-1) + [uv^2 + uv(u-1) \\ &\quad + \frac{u(u-1)(u-2)}{6}]u^n(u+2v)^{2n} \\ &\quad + (2v+u)^{n+1}(2v+u-1)[uv + \frac{u(u-1)}{2}] \\ &\quad \times \frac{u^n(2v+u)^n - (2v+u)^n}{u(2v+u) - (2v+u)}.\end{aligned}\quad (9)$$

Inserting Equation (9) into Equation (8), we obtain

$$\begin{aligned} L_{sum}(n) &= \frac{(2v+u)^{n-1}}{u(2v+u)-1} \left[\frac{3uv^2+3u^2v+u^3-u}{3} \right. \\ &\quad + \frac{[u(u-1)+2(u-2)v](2uv+u^2-1)}{2(u-1)} (2v+u)^n \\ &\quad \left. + \frac{u(u+1)[6v^2+6(u-1)v+(u-1)^2]}{6(u-1)} u^n (2v+u)^n \right]. \end{aligned} \quad (10)$$

Replacing $L_{sum}(n)$ from Equation (10) in Equation (5), we obtain

$$\begin{aligned} \langle GFPT \rangle_n &= \frac{(2v+u)^{n-1}}{[u(2v+u)-1][(2v+u)^n+1]} \left\{ \frac{6uv^2+6u^2v+2u^3-2u}{3} \right. \\ &\quad + \frac{u(u+1)[6v^2+6(u-1)v+(u-1)^2]}{3(u-1)} (2uv+u^2)^n \\ &\quad \left. + \frac{[u(u-1)+2(u-2)v](2uv+u^2-1)}{u-1} (2v+u)^n \right\}. \end{aligned} \quad (11)$$

Noticing that $N_n = (2v+u)^n + 1$ and $u^n = (N_n - 1)^{\ln u / \ln(2v+u)}$, we can rewrite Equation (11) as

$$\begin{aligned} \langle GFPT \rangle_n &= \frac{1}{[u(2v+u)-1](2v+u)} \frac{N_n-1}{N_n} \left\{ \frac{u(u+1)[6v^2+6(u-1)v+(u-1)^2]}{3(u-1)} \right. \\ &\quad \times (N_n-1)^{1+\ln u / \ln(2v+u)} + \frac{[u(u-1)+2(u-2)v](2uv+u^2-1)}{u-1} \\ &\quad \left. \times (N_n-1) + \frac{6uv^2+6u^2v+2u^3-2u}{3} \right\}. \end{aligned} \quad (12)$$

Therefore, for large networks, i.e., $n \rightarrow \infty$,

$$\langle GFPT \rangle_n \sim (N_n)^{1+\ln u / \ln(2v+u)}. \quad (13)$$

4. GMFPT for Biased Random Walk on the Weighted Fractal Scale-Free Trees

In this section, we analytically evaluate the GMFPT for biased random walks on the weighted fractal scale-free trees. At any step, the transition probability from node i to j is

$$P_{ij} = \begin{cases} \frac{w_{ij}}{\sum_{j \in v(i)} w_{ij}} & i \sim j \\ 0 & \text{otherwise} \end{cases}, \quad (14)$$

where $v(i)$ is the set of neighbors of node i , and w_{ij} is the weight of the edge between nodes i and j .

If we view the weighted fractal scale-free trees as electrical networks by considering any edge (i, j) between two adjacent nodes i and j to be a resistor with resistance $1/w_{ij}$. We find, for any $n \geq 0$, the GMFPT for biased random walks on the weighted fractal scale-free trees $G(n)$ can be expressed as [36]

$$\langle GFPT \rangle_n = \frac{F_n R_{sum}(n)}{N_n(N_n-1)}, \quad (15)$$

where $F_n = \sum_{(i \sim j)} w_{ij}$ is the sum of weights for all edges of the weighted fractal scale-free trees $G(n)$, and $R_{sum}(n) = \frac{1}{2} \sum_{i, j \in G(n), i \neq j} R_{ij}$, with R_{ij} is the the resistances between nodes i and j on $G(n)$. In order to derive $\langle GFPT \rangle_n$, we should calculate $R_{sum}(n)$ and F_n .

Firstly, we calculate $R_{sum}(n)$. It is easy to know $R_{sum}(0) = 1$. For any $n \geq 0$, as shown in Figure 4, the $G(n+1)$ is composed by $2v+u$ subunits, which are copies of $G(n)$, labeled by $G_k(n)$, $k = 1, 2, \dots, 2v+u$. Furthermore, the edge weights for subunits $G_k(n)$ ($k = 2v+1, 2v+2, \dots, 2v+u$) are the same as those of $G(n)$, whereas the weight for each edge of subunits $G_k(n)$ ($k = 1, 2, \dots, 2v$) is w times the weight for the corresponding edge of $G(n)$. We obtain

$$\begin{aligned} R_{sum}(n+1) &= \frac{1}{2} \sum_{i,j \in G(n+1), i \neq j} R_{ij} \\ &= \frac{1}{2} \sum_{k=2v+1}^{2v+u} \sum_{i,j \in G_k(n), i \neq j} R_{ij} + \frac{1}{2} r \sum_{k=1}^{2v} \sum_{i,j \in G_k(n), i \neq j} R_{ij} \\ &\quad + \frac{1}{2} \sum_{k_1 \neq k_2} \sum_{\substack{i \in G_{k_1}(n) \\ j \in G_{k_2}(n)}} R_{ij} \\ &= (2vr+u)R_{sum}(n) + \Omega_n, \end{aligned} \quad (16)$$

where $r = \frac{1}{w}$, and $\Omega_n = \frac{1}{2} \sum_{k_1 \neq k_2} \sum_{\substack{i \in G_{k_1}(n) \\ j \in G_{k_2}(n)}} R_{ij}$ is the sum of the effective resistance between

any two nodes that belong to the different subunits of $G(n+1)$.

Using Equation (16) recursively, we obtain

$$\begin{aligned} R_{sum}(n) &= (2vr+u)R_{sum}(n-1) + \Omega_{n-1} \\ &= (2vr+u)^2 R_{sum}(n-2) + (2vr+u)\Omega_{n-2} + \Omega_{n-1} \\ &= \dots \\ &= (2vr+u)^n R_{sum}(0) + \sum_{k=0}^{n-1} (2vr+u)^{n-1-k} \Omega_k. \end{aligned} \quad (17)$$

For Ω_n , we find

$$\begin{aligned} \Omega_n &= (2vr+u)^{n+1}(2v+u)^n(2v+u-1) \\ &\quad + [uv^2 + uv(u-1) + \frac{u(u-1)(u-2)}{6}]u^n(u+2v)^{2n} \\ &\quad + (2vr+u)(2v+u-1)(2v+u)^n[uv + \frac{u(u-1)}{2}] \\ &\quad \times \frac{u^n(2v+u)^n - (2vr+u)^n}{u(2v+u) - (2vr+u)}, \end{aligned} \quad (18)$$

where the detailed derivation of Equation (18) is presented in Appendix B.

Therefore, inserting Equation (18) into Equation (17), we obtain

$$\begin{aligned}
 R_{sum}(n) &= (2vr + u)^n \left[\frac{u(u^2 + 3uv + 3v^2 - 1)}{3u(2v + u)^2 - 3(2vr + u)} \right] \\
 &+ (2v + u)^n (2vr + u)^n \left[\frac{u^2 + 2uv - u - 4vr}{2u(2v + u) - 2(2vr + u)} \right] \\
 &+ u^n (2v + u)^{2n} \left\{ \frac{r(u - r)[2vr - u(u + 2v - 1)] + ur(u - 1)}{2(u - r)[2vr - u(u + 2v - 1)]} \right. \\
 &+ \frac{1}{4} + \frac{u^2 + 6vr - u}{24vr - 12u(u + 2v - 1)(u + 2v + 1)} \left. \right\} \\
 &= \left(\frac{2v}{w} + u \right)^n \left[\frac{u(u^2 + 3uv + 3v^2 - 1)}{3u(2v + u)^2 - 3\left(\frac{2v}{w} + u\right)} \right] \\
 &+ (2v + u)^n \left(\frac{2v}{w} + u \right)^n \left[\frac{uw(u + 2v - 1) - 4v}{2uw(u + 2v - 1) - 4v} \right] \\
 &+ u^n (2v + u)^{2n} \left\{ \frac{2uvw[2u^2 + 6v(v - 1) + u(6v - 3)]}{6[uw(u + 2v - 1) - 2v][uw(u^2 + 4uv + 4v^2 - 1) - 2v]} \right. \\
 &+ \frac{u^2w^2[(u + 2v - 1)(u^2 + 6uv + 6v^2 - 1)]}{6[uw(u + 2v - 1) - 2v][uw(u^2 + 4uv + 4v^2 - 1) - 2v]} \left. \right\}. \quad (19)
 \end{aligned}$$

Then, we calculate the F_n , which is the sum of weights for all edges of $G(n)$. For $n = 1$, we find $F_1 = 2(2vw + u)$. For $n > 1$, we find

$$F_n = (2vw + u)F_{n-1}. \quad (20)$$

Thus, for any $n \geq 1$,

$$F_n = 2(2vw + u)^n. \quad (21)$$

Replacing F_n and $R_{sum}(n)$ from Equations (19) and (21), respectively, we obtain

$$\begin{aligned}
 \langle GFPT \rangle_n &= \frac{F_n R_{sum}(n)}{N_n(N_n - 1)} \\
 &= \frac{2(2vw + u)^n \left(\frac{2v}{w} + u \right)^n}{(2v + u)^n [(2v + u)^n + 1]} \left[\frac{u(u^2 + 3uv + 3v^2 - 1)}{3u(2v + u)^2 - 3\left(\frac{2v}{w} + u\right)} \right] \\
 &+ \frac{2(2vw + u)^n \left(\frac{2v}{w} + u \right)^n}{(2v + u)^n + 1} \left[\frac{uw(u + 2v - 1) - 4v}{2uw(u + 2v - 1) - 4v} \right] \\
 &+ \frac{2(2vw + u)^n u^n (2v + u)^n}{(2v + u)^n + 1} \\
 &\times \left\{ \frac{2uvw[2u^2 + 6v(v - 1) + u(6v - 3)]}{6[uw(u + 2v - 1) - 2v][uw(u^2 + 4uv + 4v^2 - 1) - 2v]} \right. \\
 &+ \frac{u^2w^2[(u + 2v - 1)(u^2 + 6uv + 6v^2 - 1)]}{6[uw(u + 2v - 1) - 2v][uw(u^2 + 4uv + 4v^2 - 1) - 2v]} \left. \right\}. \quad (22)
 \end{aligned}$$

Let $w = 1$ in Equation (22), then we can recover the result, as shown in Equation (11), which is the GMFPT for the unbiased random walk on $G(n)$. Let $u = 2$ in Equation (22), then we can recover the result obtained in Ref. [36]. They all confirm the correctness of our results.

5. Optimizing the First-Passage Process by Using the GMFPT as the Measure

In this section, we analyze the effect of weight parameter w on $\langle GFPT \rangle_n$, and then find the optimal w where $\langle GFPT \rangle_n$ achieves its minimum. Therefore, we obtain a random walk strategy to speed up the first-passage process on the FSTs.

Recalling the exact result of the GMFPT, as shown in Equation (22), for a biased random walk on the weighted networks, we find for a network that is big enough, i.e., $n \rightarrow \infty$, Equation (22) can be rewritten as

$$\begin{aligned} \langle GFPT \rangle_n &\approx \frac{(2vw + u)^n}{(2v + u)^n + 1} \left\{ \frac{uw(u + 2v - 1) - 4v}{uw(u + 2v - 1) - 2v} \left(\frac{2v}{w} + u \right)^n \right. \\ &+ (2uv + u^2)^n \left\{ \frac{2uvw[2u^2 + 6v(v - 1) + u(6v - 3)]}{3[uw(u + 2v - 1) - 2v][uw(u^2 + 4uv + 4v^2 - 1) - 2v]} \right. \\ &+ \left. \left. \frac{u^2w^2[(u + 2v - 1)(u^2 + 6uv + 6v^2 - 1)]}{3[uw(u + 2v - 1) - 2v][uw(u^2 + 4uv + 4v^2 - 1) - 2v]} \right\} \right\}. \end{aligned} \quad (23)$$

Therefore, if $0 < w \leq \frac{2v}{2uv + u^2 - u}$,

$$\langle GFPT \rangle_n \sim \frac{(2vw + u)^n \left(\frac{2v}{w} + u \right)^n}{(2v + u)^n + 1}, \quad (24)$$

and if $w \geq \frac{2v}{2uv + u^2 - u}$,

$$\langle GFPT \rangle_n \sim \frac{(2vw + u)^n (2uv + u^2)^n}{(2v + u)^n + 1}. \quad (25)$$

Noticing that $N_n = (2v + u)^n + 1$, we can rewrite $\langle GFPT \rangle_n$ as

$$\langle GFPT \rangle_n \sim \begin{cases} N_n^{\frac{\ln(2vw + u) + \ln(\frac{2v}{w} + u)}{\ln(2v + u)} - 1} & 0 < w \leq \frac{2v}{2uv + u^2 - u} \\ N_n^{\frac{\ln(2uvw + u^2)}{\ln(2v + u)}} & w \geq \frac{2v}{2uv + u^2 - u} \end{cases} \quad (26)$$

Figures 5 and 6 show the double logarithmic plots of $\langle GFPT \rangle_n$ versus N_n for different choices of w in the case $u = 5, v = 2$, $u = 10, v = 2$, $u = 5, v = 5$, $u = 10$, and $v = 5$, respectively. They all confirm the asymptotic behavior in Equation (26).

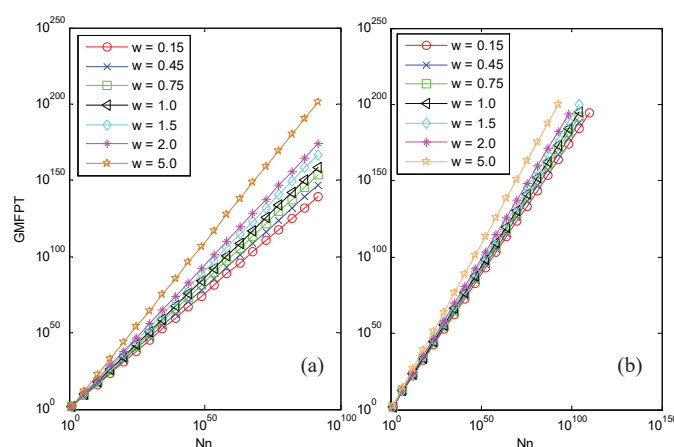


Figure 5. Double logarithmic plots of $\langle GFPT \rangle_n$ versus N_n for different choices of weight parameters w and structure parameter u and v : (a) $u = 5, v = 2$ and (b) $u = 10, v = 2$. Data for $\langle GFPT \rangle_n$ are obtained by evaluating Equation (22).

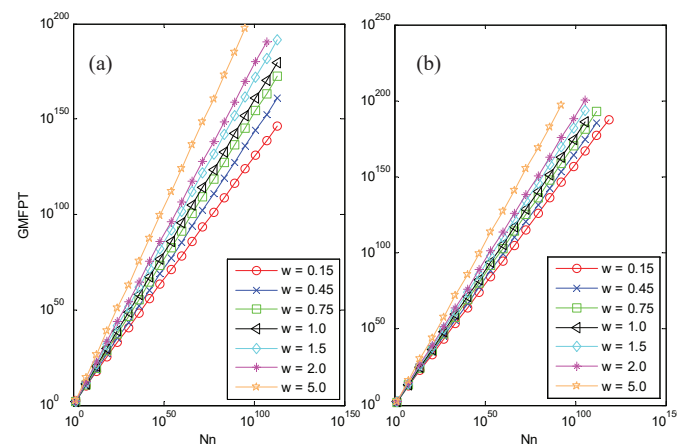


Figure 6. Double logarithmic plots of $\langle GFPT \rangle_n$ versus N_n for different choices of weight parameters w and structure parameter u and v : (a) $u = 5, v = 5$ and (b) $u = 10, v = 5$. Data for $\langle GFPT \rangle_n$ are obtained by evaluating Equation (22).

Considering the power exponent of N_n , as shown in Equation (26), one can find that $\frac{\ln(2vw+u)+\ln(\frac{2v}{w}+u)}{\ln(2v+u)} - 1$ decreases monotonically in w if $0 < w < \frac{2v}{2uv+u^2-u}$, whereas $\frac{\ln(2uvw+u^2)}{\ln(2v+u)}$ increases monotonically in w if $w > \frac{2v}{2uv+u^2-u}$. Thus, $\langle GFPT \rangle_n$ decreases monotonically as w increases if $0 < w < \frac{2v}{2uv+u^2-u}$, whereas $\langle GFPT \rangle_n$ increases monotonically in w if $w > \frac{2v}{2uv+u^2-u}$. Therefore, $\langle GFPT \rangle_n$ reaches its minimum at $w = \frac{2v}{2uv+u^2-u}$. Figures 7 and 8 shows the plots of $\langle GFPT \rangle_n$ versus w for different v in the case that $u = 3$ ($u = 5$) and $n = 60, 70$. In all the cases, $\langle GFPT \rangle_n$ reaches its minimum at $w = \frac{2v}{2uv+u^2-u}$.

Letting $w = \frac{2v}{2uv+u^2-u}$ in Equation (26), we obtained the optimal $\langle GFPT \rangle_n$, which scales as

$$\langle GFPT \rangle_{Op} \sim N_n^{\frac{\ln(u^2 + \frac{4v^2}{u+2v-1})}{\ln(2v+u)}}. \quad (27)$$

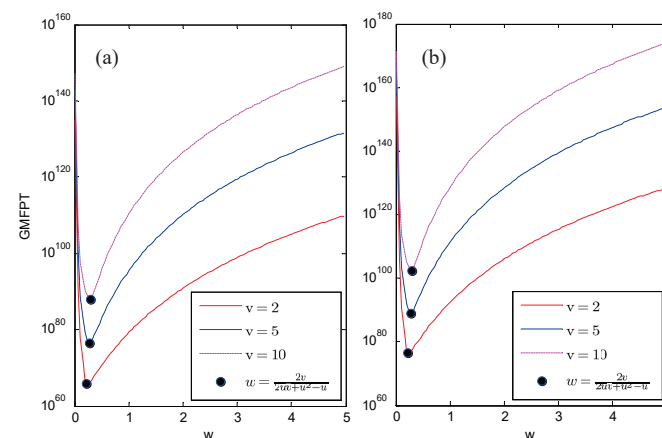


Figure 7. Plots of $\langle GFPT \rangle_n$ versus w for different v in the case $u = 3$ and (a) $n = 60$ and (b) $n = 70$. Data for $\langle GFPT \rangle_n$ are obtained by evaluating Equation (22).

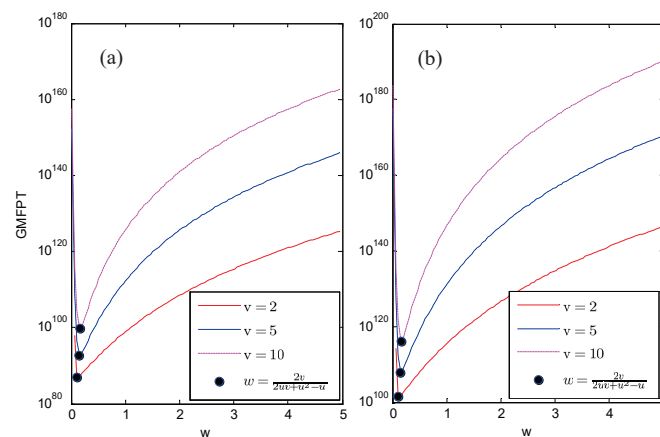


Figure 8. Plots of $\langle GFPT \rangle_n$ versus w for different v in the case $u = 5$: (a) $n = 60$ and (b) $n = 70$. Data for $\langle GFPT \rangle_n$ are obtained by evaluating Equation (22).

In order to show the improvement on the GMFPT of our optimal solution obtained here, the ratio between the optimal GMFPT $\langle GFPT \rangle_{Op}$ and the GMFPT for an unbiased random walk, as obtained in Section 3 and referred to as $\langle GFPT \rangle_{UnB}$, is evaluated, and it scales with the size of the network as

$$Ratio = \frac{\langle GFPT \rangle_{Op}}{\langle GFPT \rangle_{UnB}} \sim N_n^{\frac{\ln\left(\frac{u^2 + \frac{4v^2}{u+2v-1}}{u^2 + 2uv}\right)}{\ln(2v+u)}}. \quad (28)$$

Note that

$$u^2 + 2uv - \left(u^2 + \frac{4v^2}{u+2v-1}\right) = \frac{2v(u-1)(u+2v)}{u+2v-1} > 2v(u-1) > 2v > 0.$$

We have red $\ln\left(\frac{u^2 + \frac{4v^2}{u+2v-1}}{u^2 + 2uv}\right) < 0$, and for large networks, i.e., $N_n \rightarrow \infty$,

$$Ratio = \frac{\langle GFPT \rangle_{Op}}{\langle GFPT \rangle_{UnB}} \rightarrow 0. \quad (29)$$

Therefore, the optimal biased random walk strategy presented here shortens the GMFPT in comparison to the classical unbiased random walk strategy.

6. Conclusions

In this work, we considered a class of recursively grown networks, whose topology is controlled by two integral parameters u and v ($u \geq 2$, $v \geq 1$). These kinds of networks provide an interesting model for self-similar and scale-free networks in real life. They can also be used as a candidate structure for the artificial polymer material that has a self-similar structure with a different fractal dimension. In particular, networks in the cases of $u = 1$ and $u = 2$ constitute the formal models studied in Ref. [25].

Here, we have analytically evaluated the GMFPT for unbiased (and biased) random walks on these networks. The exact results of the GMFPT for unbiased and biased random walks are both obtained. The results show, in both cases, the GMFPTs are power functions in network size N_n .

For an unbiased random walk strategy, $\langle GFPT \rangle_n \sim (N_n)^{1+\ln u / \ln(2v+u)}$ if $u \geq 2$. For the biased random walk strategy, it is controlled by a weight parameter w ($w > 0$), and for big networks, $\langle GFPT \rangle_n$ can be looked upon as a convex function of w , which has an inflection point at $w = \frac{2v}{2uv + u^2 - u}$. Therefore, for big networks, $\langle GFPT \rangle_n$ achieves its

minimum at $w = \frac{2v}{2uv+u^2-u}$, and we obtain a way to speed up the first-passage process on fractal scale-free trees. The main reason is as follows. $\langle GFPT \rangle_n$ is proportional to the sum of effective resistances for the paths between all pairs of nodes in the network. For two arbitrary nodes, the path can be divided into two types: the first type must pass through at least one internal part, denoted by *sub-path1*, the other type does not pass through any internal parts, denoted by *sub-path2*. Then R_{sum}^1 is relevant to *sub-path1*, which is independent of w , and R_{sum}^2 is subject to parameter w . As found in Appendix B, R_{sum}^1 scales with n as $(2v+u)^n(2uv+u^2)^n$, whereas R_{sum}^2 scales with n as $(2v+u)^n(\frac{2v}{w}+u)^n$. In the asymptotic limit (i.e. $n \rightarrow \infty$), only R_{sum}^1 or R_{sum}^2 is dominant in $R_{sum}(n)$. If $(2v+u)^n(\frac{2v}{w}+u)^n < (2v+u)^n(2uv+u^2)^n$, equivalently, $w > \frac{2v}{2uv+u^2-u}$, we have $R_{sum}(n) \sim (2v+u)^n(2uv+u^2)^n$, and Equation (25) holds. On the contrary, if $w < \frac{2v}{2uv+u^2-u}$, we have $R_{sum}(n) \sim (2v+u)^n(\frac{2v}{w}+u)^n$, and Equation (24) holds. Therefore, $w = \frac{2v}{2uv+u^2-u}$ is just the inflection point of $\langle GFPT \rangle_n$ with respect to w .

The results obtained here provide interesting hints for the design of a polymer embedding diffusion process. First, one can construct a class of polymers with different fractal dimensions and different transport efficiencies. The bigger the fractal dimension, the slower the transport on the networks. One can also improve the transport efficiency of the polymer by properly adjusting the weights of each edge.

In future research, we can also set the weight which is related to the node degree, for example, $w_{ij} = \frac{1}{d_i} + \frac{1}{d_j}$, where d_i and d_j is the degree of node i, j . How we to optimize the first-passage process in this case is an interesting problem.

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Abbreviations

The following abbreviations are used in this manuscript:

MDPI	Multidisciplinary Digital Publishing Institute
DOAJ	Directory of open access journals
TLA	Three letter acronym
LD	Linear dichroism

Appendix A. Derivation of Equation (9)

In this appendix, we present the detailed derivation of Δ_n , which is the sum of the shortest path length for any two nodes that belong to the different subunits of $G(n+1)$. As shown in Figure 3, the fractal scale-free trees of generation $n+1$, denoted by $G(n+1)$, is composed of $2v+u$ subunits, labeled by $G_k(n)$ ($k=1, 2, \dots, 2v+u$), which are connected to one another by their hubs (i.e., nodes A, B and $O_m, m=1, 2, \dots, u-1$). For convenience, we call the subunits $G_k(n)$ ($k=1, 2, \dots, 2v$) as the exterior subunits of $G(n+1)$ and sub-

units $G_k(n)$ ($k = 2v + 1, 2v + 2, \dots, 2v + u$) as the internal subunits of $G(n + 1)$. For any $k_1 \neq k_2$ ($k_1, k_2 = 1, 2, \dots, 2v + u$), let

$$\Delta_n^{k_1, k_2} = \sum_{\substack{i \in G_{k_1}(n) \\ j \in G_{k_2}(n)}} L_{ij} \quad (A1)$$

denote the sum of the shortest path between any node in subunit $G_{k_1}(n)$ and any node in subunit $G_{k_2}(n)$. We have

$$\begin{aligned} \Delta_n &= \frac{1}{2} \sum_{k_1 \neq k_2} \sum_{\substack{i \in G_{k_1}(n) \\ j \in G_{k_2}(n)}} L_{ij} \\ &= \sum_{k_1=1}^v \sum_{k_2=k_1+1}^v \Delta_n^{k_1, k_2} + \sum_{k_1=v+1}^{2v} \sum_{k_2=k_1+1}^{2v} \Delta_n^{k_1, k_2} \\ &\quad + \sum_{k_1=1}^v \sum_{k_2=2v+1}^{2v+u} \Delta_n^{k_1, k_2} + \sum_{k_1=v+1}^{2v} \sum_{k_2=2v+1}^{2v+u} \Delta_n^{k_1, k_2} \\ &\quad + \sum_{k_1=2v+1}^{2v+u} \sum_{k_2=k_1+1}^{2v+u} \Delta_n^{k_1, k_2} + \sum_{k_1=1}^v \sum_{k_2=v+1}^{2v} \Delta_n^{k_1, k_2}. \end{aligned} \quad (A2)$$

Noticing the symmetry of network topology, we have

$$\sum_{k_1=1}^v \sum_{k_2=k_1+1}^v \Delta_n^{k_1, k_2} = \sum_{k_1=v+1}^{2v} \sum_{k_2=k_1+1}^{2v} \Delta_n^{k_1, k_2},$$

and

$$\begin{aligned} &\sum_{k_1=1}^v \sum_{k_2=k_1+1}^v \Delta_n^{k_1, k_2} \\ &= \frac{(v^2 - v)}{2} \Delta_n^{1,2} \\ &= \frac{(v^2 - v)}{2} \sum_{\substack{i \in G_1(n), j \in G_2(n) \\ i, j \neq A}} L_{ij}(n) \\ &= \frac{(v^2 - v)}{2} \sum_{\substack{i \in G_1(n), j \in G_2(n) \\ i, j \neq A}} [L_{iA}(n) + L_{jA}(n)] \\ &= \frac{(v^2 - v)}{2} \{ (N_n - 1) \sum_{i \in G_1(n), i \neq A} L_{iA} + (N_n - 1) \sum_{i \in G_2(n), i \neq A} L_{iA} \} \\ &= (v^2 - v)(N_n - 1)S_n, \end{aligned} \quad (A3)$$

where N_n is the total number of nodes of $G(n)$ and

$$S_n = \sum_{i \in G(n), i \neq A} L_{iA}. \quad (A4)$$

Thus,

$$\sum_{k_1=1}^v \sum_{k_2=k_1+1}^v \Delta_n^{k_1, k_2} + \sum_{k_1=v+1}^{2v} \sum_{k_2=k_1+1}^{2v} \Delta_n^{k_1, k_2} = 2(v^2 - v)(N_n - 1)S_n. \quad (A5)$$

Similarly,

$$\begin{aligned}
 & \sum_{k_1=1}^v \sum_{k_2=2v+1}^{2v+u} \Delta_n^{k_1, k_2} \\
 &= v \sum_{k_2=2v+1}^{2v+u} \Delta_n^{1, k_2} \\
 &= v(\Delta_n^{1, 2v+1} + \Delta_n^{1, 2v+2} + \dots + \Delta_n^{1, 2v+u}),
 \end{aligned} \tag{A6}$$

and for any $m = 1, 2, \dots, u$,

$$\begin{aligned}
 \Delta_n^{1, 2v+m} &= \sum_{\substack{i \in G_1(n), i \neq A \\ j \in G_{2v+m}(n), j \neq O_{m-1}}} L_{ij}(n) \\
 &= \sum_{\substack{i \in G_1(n), i \neq A \\ j \in G_{2v+m}(n), j \neq O_{m-1}}} [L_{iA}(n) + L_{AO_{m-1}}(n) + L_{jO_{m-1}}(n)] \\
 &= 2(N_n - 1)S_n + (m - 1)u^n(N_n - 1)^2,
 \end{aligned} \tag{A7}$$

where node O_{m-1} represents node A , while $m = 1$. Thus,

$$\begin{aligned}
 \sum_{k_1=1}^v \sum_{k_2=2v+1}^{2v+u} \Delta_n^{k_1, k_2} &= v(\Delta_n^{1, 2v+1} + \Delta_n^{1, 2v+2} + \dots + \Delta_n^{1, 2v+u}) \\
 &= v[2(N_n - 1)S_n + 2(N_n - 1)S_n + u^n(N_n - 1)^2 \\
 &\quad + \dots + 2(N_n - 1)S_n + (u - 1)u^n(N_n - 1)^2] \\
 &= v[2u(N_n - 1)S_n + u^n(N_n - 1)^2(1 + 2 + \dots + u - 1)] \\
 &= 2uv(N_n - 1)S_n + \frac{uv(u - 1)}{2}u^n(N_n - 1)^2.
 \end{aligned} \tag{A8}$$

By symmetry,

$$\begin{aligned}
 & \sum_{k_1=1}^v \sum_{k_2=2v+1}^{2v+u} \Delta_n^{k_1, k_2} + \sum_{k_1=v+1}^{2v} \sum_{k_2=2v+1}^{2v+u} \Delta_n^{k_1, k_2} \\
 &= 4uv(N_n - 1)S_n + uv(u - 1)u^n(N_n - 1)^2.
 \end{aligned} \tag{A9}$$

Similarly,

$$\begin{aligned}
 \Delta_n^{1, v+1} &= \sum_{\substack{i \in G_1(n), i \neq A \\ j \in G_{v+1}(n), j \neq B}} L_{ij}(n) \\
 &= \sum_{\substack{i \in G_1(n), i \neq A \\ j \in G_{v+1}(n), j \neq B}} [L_{iA}(n) + L_{AB}(n) + L_{jB}(n)] \\
 &= 2(N_n - 1)S_n + u^{n+1}(N_n - 1)^2,
 \end{aligned} \tag{A10}$$

and

$$\begin{aligned}
 \Delta_n^{2v+1, 2v+m} &= \sum_{\substack{i \in G_{2v+1}(n), i \neq O_1 \\ j \in G_{2v+m}(n), j \neq O_{m-1}}} L_{ij}(n) \\
 &= \sum_{\substack{i \in G_{2v+1}(n), i \neq O_1 \\ j \in G_{2v+m}(n), j \neq O_{m-1}}} [L_{iO_1}(n) + L_{O_1O_{m-1}}(n) + L_{jO_{m-1}}(n)] \\
 &= 2(N_n - 1)S_n + (m - 2)u^n(N_n - 1)^2,
 \end{aligned} \tag{A11}$$

where $m = 2, 3, \dots, u$. Therefore, we have

$$\begin{aligned} \sum_{k_1=1}^v \sum_{k_2=v+1}^{2v} \Delta_n^{k_1, k_2} &= v^2 \Delta_n^{1, v+1} \\ &= 2v^2(N_n - 1)S_n + v^2 u^{n+1}(N_n - 1)^2, \end{aligned} \quad (\text{A12})$$

and

$$\begin{aligned} \sum_{k_1=2v+1}^{2v+u} \sum_{k_2=k_1+1}^{2v+u} \Delta_n^{k_1, k_2} &= \sum_{m=2}^u (u - m + 1) \Delta_n^{2v+1, 2v+m} \\ &= (u - 1) \Delta_n^{2v+1, 2v+2} + (u - 2) \Delta_n^{2v+1, 2v+3} + \dots + \Delta_n^{2v+1, 2v+u} \\ &= 2(N_n - 1)S_n[(u - 1) + (u - 2) + \dots + 1] \\ &\quad + [(u - 2) + 2(u - 3) + \dots + (u - 2)]u^n(N_n - 1)^2 \\ &= u(u - 1)(N_n - 1)S_n + \frac{u(u - 1)(u - 2)}{6}u^n(N_n - 1)^2. \end{aligned} \quad (\text{A13})$$

Inserting Equations (A5), (A9), (A12) and (A13) into Equation (A2), we obtain

$$\begin{aligned} \Delta_n &= (2v + u)(2v + u - 1)(N_n - 1)S_n \\ &\quad + [uv^2 + uv(u - 1) + \frac{u(u - 1)(u - 2)}{6}]u^n(N_n - 1)^2. \end{aligned} \quad (\text{A14})$$

For S_n , for any $n > 1$, S_n satisfies the following recursion relation:

$$\begin{aligned} S_n &= (v + 1)S_{n-1} + \sum_{m=1}^{u-1} [S_{n-1} + mu^{n-1}(N_{n-1} - 1)] + v[S_{n-1} + u^n(N_{n-1} - 1)] \\ &= (2v + u)S_{n-1} + [uv + \frac{u(u - 1)}{2}]u^{n-1}(2v + u)^{n-1}, \end{aligned} \quad (\text{A15})$$

with the initial condition $S_0 = 1$. By solving the recursion relation, we obtain

$$S_n = (2v + u)^n + [uv + \frac{u(u - 1)}{2}] \times \frac{u^n(2v + u)^n - (2v + u)^n}{u(2v + u) - (2v + u)}. \quad (\text{A16})$$

Plugging Equations (3) and (A16) into Equation (A14), we obtain Equation (9).

Appendix B. Derivation of Equation (18)

In this part, we present the detailed derivation of Ω_n , which is the sum of the effective resistance between For any $k_1 \neq k_2$ ($k_1, k_2 = 1, 2, \dots, 2v + u$), let

$$\Omega_n^{k_1, k_2} = \sum_{\substack{i \in G_{k_1}(n) \\ j \in G_{k_2}(n)}} R_{ij} \quad (\text{A17})$$

denote the sum of resistance between any node i of subunit $G_{k_1}(n)$ and any node j of subunit $G_{k_2}(n)$. We have

$$\begin{aligned}
 \Omega_n &= \frac{1}{2} \sum_{k_1 \neq k_2} \sum_{\substack{i \in G_{k_1}(n) \\ j \in G_{k_2}(n)}} R_{ij} \\
 &= \sum_{k_1=1}^v \sum_{k_2=k_1+1}^v \Omega_n^{k_1, k_2} + \sum_{k_1=v+1}^{2v} \sum_{k_2=k_1+1}^{2v} \Omega_n^{k_1, k_2} \\
 &+ \sum_{k_1=1}^v \sum_{k_2=2v+1}^{2v+u} \Omega_n^{k_1, k_2} + \sum_{k_1=v+1}^{2v} \sum_{k_2=2v+1}^{2v+u} \Omega_n^{k_1, k_2} \\
 &+ \sum_{k_1=2v+1}^{2v+u} \sum_{k_2=k_1+1}^{2v+u} \Omega_n^{k_1, k_2} + \sum_{k_1=1}^v \sum_{k_2=v+1}^{2v} \Omega_n^{k_1, k_2}. \quad (\text{A18})
 \end{aligned}$$

Similar to the derivation of Equation (9), we find

$$\begin{aligned}
 &\sum_{k_1=1}^v \sum_{k_2=k_1+1}^v \Omega_n^{k_1, k_2} + \sum_{k_1=v+1}^{2v} \sum_{k_2=k_1+1}^{2v} \Omega_n^{k_1, k_2} \\
 &= (v^2 - v) \Omega_n^{1,2} \\
 &= (v^2 - v) \sum_{\substack{i \in G_1(n), j \in G_2(n) \\ i, j \neq A}} R_{ij}(n) \\
 &= (v^2 - v) \sum_{\substack{i \in G_1(n), j \in G_2(n) \\ i, j \neq A}} [R_{iA}(n) + R_{jA}(n)] \\
 &= (v^2 - v) \left[(N_n - 1) \sum_{i \in G_1(n), i \neq A} R_{iA} + (N_n - 1) \sum_{j \in G_2(n), j \neq A} R_{jA} \right] \\
 &= 2r(v^2 - v)(N_n - 1) \mathfrak{R}_n, \quad (\text{A19})
 \end{aligned}$$

where N_n is the total number of nodes of $G(n)$ and

$$\mathfrak{R}_n = \sum_{i \in G(n), i \neq A} R_{iA}. \quad (\text{A20})$$

Similarly,

$$\begin{aligned}
 &\sum_{k_1=1}^v \sum_{k_2=2v+1}^{2v+u} \Omega_n^{k_1, k_2} + \sum_{k_1=v+1}^{2v} \sum_{k_2=2v+1}^{2v+u} \Omega_n^{k_1, k_2} \\
 &= 2v \sum_{k_2=2v+1}^{2v+u} \Omega_n^{1, k_2} \\
 &= 2v(\Omega_n^{1, 2v+1} + \Omega_n^{1, 2v+2} + \dots + \Omega_n^{1, 2v+u}), \quad (\text{A21})
 \end{aligned}$$

and

$$\begin{aligned}
 \Omega_n^{1, 2v+m} &= \sum_{\substack{i \in G_1(n), i \neq A \\ j \in G_{2v+m}(n), j \neq O_{m-1}}} R_{ij}(n) \\
 &= \sum_{\substack{i \in G_1(n), i \neq A \\ j \in G_{2v+m}(n), j \neq O_{m-1}}} [R_{iA}(n) + R_{AO_{m-1}}(n) + R_{jO_{m-1}}(n)] \\
 &= (r+1)(N_n - 1) \mathfrak{R}_n + (m-1)u^n(N_n - 1)^2. \quad (\text{A22})
 \end{aligned}$$

Thus, we obtain

$$\begin{aligned}
 & \sum_{k_1=1}^v \sum_{k_2=2v+1}^{2v+u} \Omega_n^{k_1, k_2} + \sum_{k_1=v+1}^{2v} \sum_{k_2=2v+1}^{2v+u} \Omega_n^{k_1, k_2} \\
 &= 2v(\Omega_n^{1, 2v+1} + \Omega_n^{1, 2v+2} + \dots + \Omega_n^{1, 2v+u}) \\
 &= 2v[(r+1)(N_n-1)\mathfrak{R}_n + (r+1)(N_n-1)\mathfrak{R}_n + u^n(N_n-1)^2 \\
 &+ \dots + (r+1)(N_n-1)\mathfrak{R}_n + (u-1)u^n(N_n-1)^2] \\
 &= 2v[u(r+1)(N_n-1)\mathfrak{R}_n + u^n(N_n-1)^2(1 + \dots + u-1)] \\
 &= 2uv(r+1)(N_n-1)\mathfrak{R}_n + uv(u-1)u^n(N_n-1)^2. \tag{A23}
 \end{aligned}$$

We also find

$$\begin{aligned}
 \sum_{k_1=2v+1}^{2v+u} \sum_{k_2=k_1+1}^{2v+u} \Omega_n^{k_1, k_2} &= (u-1)\Omega_n^{2v+1, 2v+2} + (u-2)\Omega_n^{2v+1, 2v+3} + \dots + \Omega_n^{2v+1, 2v+u} \\
 &= 2(N_n-1)\mathfrak{R}_n[(u-1) + (u-2) + \dots + 1] \\
 &+ [(u-2) + 2(u-3) + \dots + (u-2)]u^n(N_n-1)^2 \\
 &= u(u-1)(N_n-1)\mathfrak{R}_n + \frac{u(u-1)(u-2)}{6}u^n(N_n-1)^2, \tag{A24}
 \end{aligned}$$

and

$$\begin{aligned}
 \Omega_n^{1, v+1} &= \sum_{\substack{i \in G_1(n), i \neq A \\ j \in G_{v+1}(n), j \neq B}} R_{ij}(n) \\
 &= \sum_{\substack{i \in G_1(n), i \neq A \\ j \in G_{v+1}(n), j \neq B}} [R_{iA}(n) + R_{AB}(n) + R_{jB}(n)] \\
 &= 2r(N_n-1)\mathfrak{R}_n + u^{n+1}(N_n-1)^2. \tag{A25}
 \end{aligned}$$

Thus,

$$\begin{aligned}
 \sum_{k_1=1}^v \sum_{k_2=v+1}^{2v} \Omega_n^{k_1, k_2} &= v^2 \Omega_n^{1, v+1} \\
 &= 2v^2 r(N_n-1)\mathfrak{R}_n + v^2 u^{n+1}(N_n-1)^2. \tag{A26}
 \end{aligned}$$

Inserting Equations (A19), (A23), (A24) and (A26) into Equation (A2), we obtain

$$\begin{aligned}
 \Omega_n &= (2vr+u)(2v+u-1)(N_n-1)\mathfrak{R}_n \\
 &+ [uv^2 + uv(u-1) + \frac{u(u-1)(u-2)}{6}]u^n(N_n-1)^2. \tag{A27}
 \end{aligned}$$

Similarly, for \mathfrak{R}_n , for any $n \geq 0$, \mathfrak{R}_n satisfies the following recursion relation:

$$\begin{aligned}
 \mathfrak{R}_n &= vr\mathfrak{R}_{n-1} + \sum_{m=1}^u [\mathfrak{R}_{n-1} + (m-1)u^{n-1}(N_{n-1}-1)] \\
 &+ v[r\mathfrak{R}_{n-1} + u^n(N_{n-1}-1)] \\
 &= (2vr+u)\mathfrak{R}_{n-1} + [uv + \frac{u(u-1)}{2}]u^{n-1}(2v+u)^{n-1}, \tag{A28}
 \end{aligned}$$

with the initial condition $\mathfrak{R}_0 = 1$. By solving the Equation (A28), we obtain

$$\mathfrak{R}_n = (2vr+u)^n + [uv + \frac{u(u-1)}{2}][\frac{u^n(2v+u)^n - (2vr+u)^n}{u(2v+u) - (2vr+u)}]. \tag{A29}$$

Plugging Equations (A29) and (3) into Equation (A27), we get Equation (18).

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