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Mean first passage time for random walk on dual structure of dendrimer

Ling Li [a,b], Jihong Guan [a,*], Shuigeng Zhou [c,d]

[a] Department of Computer Science and Technology, Tongji University, 4800 Caoan Road, Shanghai 201804, China
[b] Basic Courses Department, Zhejiang Shuren University, Hangzhou 310015, China
[c] School of Computer Science, Fudan University, Shanghai 200433, China
[d] Shanghai Key Lab of Intelligent Information Processing, Fudan University, Shanghai 200433, China

HIGHLIGHTS

- We determine the partial and global MFPT of random walks on dual dendrimers.
- We uncover the impact of trap location on the transport efficiency on dual dendrimers.
- We discuss the influence of loop structure on the transport efficiency.

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ABSTRACT

The random walk approach has recently been widely employed to study the relations between the underlying structure and dynamic of complex systems. The mean first-passage time (MFPT) for random walks is a key index to evaluate the transport efficiency in a given system. In this paper we study analytically the MFPT in a dual structure of dendrimer network, Husimi cactus, which has different application background and different structure (contains loops) from dendrimer. By making use of the iterative construction, we explicitly determine both the partial mean first-passage time (PMFT, the average of MFPTs to a given target) and the global mean first-passage time (GMFT, the average of MFPTs over all couples of nodes) on Husimi cactus. The obtained closed-form results show that PMFPT and EMFPT follow different scaling with the network order, suggesting that the target location has essential influence on the transport efficiency. Finally, the impact that loop structure could bring is analyzed and discussed.

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1. Introduction

Networks have gained recognitions as a kind of fundamental representation of various complex systems; including physics, biological system, the Internet, social system and many others [1–5]. Structure and dynamics are two important issues in network studies. Accordingly, it becomes a basic challenge to understand the relations between the underlying topology of the system and its dynamics [3,6]. As a representative stochastic process, random walks have been introduced into complex networks to simulate a wide variety of dynamics in distinct fields [7,8]. The most useful quantity in the analysis of random walk is mean first-passage time (MFPT), which is the expected number of steps before the target node is

* Corresponding author. Tel.: +86 2165109899.
E-mail address: jhguan@tongji.edu.cn (J. Guan).

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visited as starting from a source node [9–12]. MFPT provides a quantitative standard for measuring the transport efficiency of random walks, and is proven to be closely related to various dynamical processes in complex system, e.g. page access and search in internet [13–16], lighting harvesting in cell [17,18]. A lot of activities have been devoted to calculating MFPT for a lot of systems, such as regular lattices [19], the treelike T-fractals [20–22], the small world networks [23,24] and the modular scale free graph [25,26].

According to the choice of starting node and the target node, those previous works about MFPT can be grouped into several situations. For instance, the case of a fixed starting node [27,28] and the case of a given target node [29]. We focus on the latter case in this paper, known as the partial mean first-passage time (PMFPT) when the target node is fixed and the global mean first-passage time (GMFPT) when the target node is located uniformly. Since MFPT is also known as trapping time (TT) when considering the target node as a trap [19] (which will absorb all walkers that visit it). We will use trap and trapping time to describe the problem of random walk and MFPT below, respectively.

The past decades has witnessed an almost explosive development of polymer physics. As a representative network, dendrimer (also called Cayley tree) [30–34] has extensive applications in different fields, including medicinal and diagnosis [35,36], drug delivery system [37,38], light harvesting [39,40] and electronic applications [41]. Random walks on dendrimer have been widely studied [42–45]. During the transport processes, the excitations are usually located on the chromophores of dendrimer or the segments connecting the chromophores [46]. In the latter case, the underlying topology turns into the dual structure of the dendrimer, which is derived by replacing each edge of the dendrimer by a node and connecting nodes that represent adjacent edges in the corresponding dendrimer (as in Fig. 1). This structure is called Husimi cactus [47]. Some authors have focused their attention on Husimi cactus and made many efforts, e.g. determining the complete spectra of the network to study the dynamics on it [48,49], calculating the entropy of polydisperse chains placed on the structure [50], studying the discrete-time quantum walk-based search for a marked vertex [51], exploring continuous-time quantum walks on Husimi cacti and comparing with results on dendrimer [52], and solving a model of interacting self-avoiding walks [53]. In this work, we will focus on trapping process on Husimi cactus. Besides, the major difference between the structures of dendrimer and Husimi cactus is that the former is a tree while the latter contains loops. The previous research showed that the existence of loops has strong correlation with the dynamics of polymer networks [54–56], so that we also analyze the influence of loop structure on trapping process by comparing the results of Husimi cactus with dendrimer.

The organization of this paper is as follows: in Section 2 we introduce the construction and some properties of Husimi cacti. As previously mentioned, we study in Section 3 the random walk problem with a trap fixed at one of the central nodes, and average over all possible starting nodes to obtain the exact formula of PMFPT to the trap. In Section 4 we turn to discuss the case that the trap is uniformly selected among all nodes and derive the solution to GMFPT between all pairs of nodes. From the results, we give the dependence relation of MFPT on the network order. Section 5 will conclude this paper.

2. Brief introduction to Husimi cactus

The Husimi cactus is the dual structure of a dendrimer (Cayley tree). So we introduce the construction of Cayley tree first. From a central node emerge m branches, each of which ends with a new node. Then from each of these new nodes, another $m-1$ branches are created. Calling the central node the generation 0, one can perform iteratively from generation $g-1$ to generation g for any $g>1$. Once given a Cayley tree, we can achieve a Husimi cactus by replacing each edge with a node, and connecting all the nodes adjacent to each dendrimer node through a new edge. Let $H_{m,g}$ ($m\geq 3, g\geq 1$) denote the Husimi cactus after g iteration. Fig. 1 illustrates the construction process for a particular Husimi cactus, $H_{3,5}$. Obviously, distinct from dendrimers which are trees, the Husimi cacti have loops. For simplicity, we will discuss in detail the Husimi cactus with $m=3$ (also called triangular Husimi cactus) in this paper and use H_g to represent Husimi cactus alternatively.

Notice that in addition to dual graphs of dendrimers, Husimi cactus can be alternatively constructed in another approach. Initially ($g=1$), H_1 is a triangle, in which there is a connection between each pair of nodes. Then H_g ($g>1$) can be obtained from H_{g-1} as follows. For each outermost node (with its degree equals to 2) in H_{g-1}, two new nodes are created and linked to the old one. Then we call the old node "parent" node, and two new nodes are named "child" nodes. And there is also an edge introduced into the network to link the two child nodes.

By the construction, we categorize the nodes in H_g into g levels according to the priority of their appearance. The original three nodes (labeled with 1, 2 and 3 in Fig. 1) are at level 1, and the nodes generated at generation 2 are at level 2, and so on. Furthermore, all the nodes in H_g can be divided into three branches (denoted by $H_g^{(k)}$, $k=1,2,3$) on their earliest ancestor (as illustrated in Fig. 2). The original three nodes can be considered as root nodes of each branch and different branches communicated through the connections between these root nodes. The second construction method emphasized the hierarchical structure and self-similarity of Husimi cactus.

In light of the construction, there are $\widehat{N}(i)=3\times 2^{i-1}$ nodes (2^{i-1} ones in each branch) newly created at generation i. Therefore the total number of nodes in H_g is

$$N_g=\sum_{i=1}^{g}\widehat{N}(i)=3(2^g-1). \tag{1}$$

At the same time, each node created in generation $i-1$ produces three new edges in generation i ($i>1$). Thus the number of newly created edges in iteration i is $\widehat{E}(i)=3\widehat{N}(i-1)=9\times 2^{i-2}$, and one can easily calculate out the total number of

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