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Coalescent random walks on graphs

Jianjun Paul Tian[a,*], Zhenqiu Liu[b]

[a] *Mathematical Biosciences Institute, The Ohio State University, 18th Avenue, Columbus OH 43210, USA*
[b] *Division of Biostatistics, Greenebaum Cancer Center and Department of Epidemiology and Preventive Medicine, University of Maryland Medicine, USA*

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Abstract

Inspired by coalescent theory in biology, we introduce a stochastic model called "multi-person simple random walks" or "coalescent random walks" on a graph G. There are any finite number of persons distributed randomly at the vertices of G. In each step of this discrete time Markov chain, we randomly pick up a person and move it to a random adjacent vertex. To study this model, we introduce the tensor powers of graphs and the tensor products of Markov processes. Then the coalescent random walk on graph G becomes the simple random walk on a tensor power of G. We give estimates of expected number of steps for these persons to meet all together at a specific vertex. For regular graphs, our estimates are exact.

1. Introduction

Inspired by coalescent theory in population genetics, we consider, in the present paper, a class of models, called coalescent random walks on graphs which is actually an generalization of coalescent theory. Let us recall the basic idea about coalescent theory firstly. Taking a sample with n individuals from a population, we label them as $1, 2, \ldots, n$, and ask a question how long ago the recent common ancestor of the sample lived. Coalescent theory answers this question by running a continuous time Markov chain over the collection of partitions $A_1, A_2, \ldots, A_t$ of $1, 2, \ldots, n$, where each A_i consists of one subset of individuals that have coalesced and hence are identical by descent. To explain this theory, we look at an example that the sample consists of five individuals $1, 2, \ldots, 5$. For the purpose of illustration, we randomly choose partitions at each time when a coalescent event happens. As we work backwards in time, partitions were chosen as the following:

time	0	$\{1\}$	$\{2\}$	$\{3\}$	$\{4\}$	$\{5\}$
	T_4	$\{1, 2\}$	$\{3\}$	$\{4\}$	$\{5\}$	
	T_3	$\{1, 2\}$	$\{3\}$	$\{4, 5\}$		
	T_2	$\{1, 2, 3\}$	$\{4, 5\}$			
	T_1	$\{1, 2, 3, 4, 5\}$.				

Initially, the partition consists of five singletons since there has been no coalescence. After 1 and 2 coalesce at time T_4, they appear in the same set. Then 4 and 5 coalesce at time T_3, etc. Finally, at time T_1 we end up with all the labels

* Corresponding author.
E-mail address: tianjj@mbi.osu.edu (J.P. Tian).

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in one set. After figured out the probabilities of coalescent events, Kingman [5,6] got a continuous time Markov chain asymptotically. That is coalescent theory. If we construct a graph by taking the set of vertices as the set of all partitions of labeled individuals of a sample and the set of edges as the set of coalescent relations, we could see that coalescent theory is a class of continuous time Markov chains over a special class of graphs. The graphs are special, because they have a kind of partial directions from n distinct vertices to the other one vertex which represent the genealogical relations. From a different viewpoint, coalescent theory models how n particles come together under certain conditions. Therefore, we generally consider the following model that we call k-coalescent random walks or multi-person simple random walks.

Given a graph G with n vertices and m edges, and suppose that k persons distribute on n vertices of G. We here allow that several persons can stand together on one vertex and k can be bigger than n or smaller than n. At each time step, one person could randomly move to one of his neighbor vertices with the equal probability of moving any one of his neighbor vertices except the vertex he currently stands on. Then, there arises an interesting question that when these k persons will first time meet together on a specific vertex.

To solve this problem, in the rest of the article, we generalize the concept of the tensor powers of a graph, which are introduced in paper [9]. We recall the tensor products of Markov processes. By using the continuous time Markov chains over the kth tensor powers of the given graph, we turn the k-coalescent random walks on the ground graph G into the simple random walks on its kth tensor powers. This way, we get an estimation of the expectation of the time steps that k persons starting with any distribution on the graph come together at a specific vertex.

For simplicity, we only consider connected simple graphs. These are connected graphs without multiple edges and loops. We adopt the following notations and terminologies for a graph G. The sets of vertices and edges of G are $V(G)$ and $E(G)$, respectively. The *order* n of G is the number of vertices of G, and the *size* m of G is the number of edges of G. Thus, $n = |V(G)|$ and $m = |E(G)|$. For a vertex $x \in V(G)$, $\Gamma(x)$ is the set of vertices which are connected to x by an edge in $E(G)$. The *degree* of a vertex x is $d(x) = |\Gamma(x)|$. We have

$$\sum_{x \in V(G)} d(x) = 2m.$$

The adjacent matrix of G is denote by $A(G)$ and the diagonal matrix $D(G)$ has the sequence of degrees at each vertex as its diagonal entries. Finally, we denote

$$d_m = \min\{d(x); x \in V(G)\} \quad \text{and} \quad d_M = \max\{d(x); x \in V(G)\}.$$

We would like to refer the reader to [7,1,9,3] for basic notions and results in the study of simple random walks on graphs.

2. Coalescent random walks and simple random walks on graphs

2.1. The tensor powers of graphs

For a graph G with order n and size m, a nth tensor power of G was introduced in paper [9]. It is not necessary to constrain the order of tensor power to be the order of the graph. Although the motivation of our generalization of tensor powers of a graph is coalescent random walks of any number of persons on the graph, the general tensor powers have their own interesting applications.

Let I_k and I_n be finite sets of cardinalities k and n, respectively. For example, we may have $I_k = \{1, 2, \ldots, k\}$, and $I_n = \{1, 2, \ldots, n\}$. We denote the set of all maps from I_k to I_n by $M_{k,n}$. When $k = n$, we have the symmetric group S_n sitting inside of $M_{n,n}$. A map $x \in M_{k,n}$ is called a *generalized permutation of deficiency* j if

$$|x(I_k)| = k - j.$$

We denote $\operatorname{def}(x) = j$.

$M_{k,n}$ is a semigroup under composition when $k \geqslant n$. The symmetrical group S_n is a subgroup of $M_{k,n}$ only when $k = n$. The deficiency determines a grading on $M_{k,n}$ which is compatible with the semigroup product on $M_{k,n}$:

$$\operatorname{def}(x) + \operatorname{def}(y) \geqslant 2\operatorname{def}(x \circ y).$$

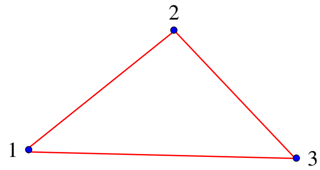

Fig. 1. The ground graph G.

Denote $M_{k,n}^{(j)} = \{\text{all maps with deficiency } j\}$, then we have a decomposition of $M_{k,n}$ according to the deficiency

$$M_{k,n} = M_{k,n}^{(k-n)} \amalg M_{k,n}^{(k-n+1)} \amalg M_{k,n}^{(k-n+2)} \amalg \cdots \amalg M_{k,n}^{(k-1)},$$

where $M_{k,n}^{(k-n)}$ is the set of all surjective maps. $M_{k,n}$ has a similar decomposition when $k \leqslant n$. That is,

$$M_{k,n} = M_{k,n}^{(0)} \amalg M_{k,n}^{(1)} \amalg M_{k,n}^{(2)} \amalg \cdots \amalg M_{k,n}^{(k-1)},$$

where $M_{k,n}^{(0)}$ is the set of all injective maps.

We identify the set of vertices $V(G)$ of graph G with I_n, and we call G the ground graph. Let the adjacent matrix $A(G) = (a_{ij})_{n\times n}$ with entries given by

$$a_{ij} = \begin{cases} 1 & \text{if } ij \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

For any positive integer k, we define a new graph $M_{k,n}(G)$ which we call the kth tensor power of G as follows. $V(M_{k,n}(G)) = M_{k,n}$, that is, the set of vertices of $M_{k,n}(G)$ is the set of all maps from I_k to I_n; For $x, y \in M_{k,n}$, there is an edge xy in $M_{k,n}(G)$ only when

$$|\{i : x(i) \neq y(i)\}| = 1,$$

and if $x(i) \neq y(i)$, then $A_{xy} = a_{x(i)y(i)} = 1$, where A_{xy}'s are the entries of the adjacent matrix of $M_{k,n}(G)$.

It is easy to see that the order of $M_{k,n}(G)$ is n^k. However, the degrees of vertices and size of $M_{k,n}(G)$ are not easy to compute directly. They will become corollaries after we connect the coalescent random walks on G and the simple random walks on $M_{k,n}(G)$. We here give an example to see how to construct a tensor power of a ground graph. The ground graph is a triangle G, a regular graph with degree 2. We denote its vertices by numbers 1, 2 and 3 (Fig. 1).

We look at the third tensor power which has order 27 and size 81. Notice that the number sequence on a vertex represents the map from I_3 to I_3. For instant, 232 represents the map that send 1 to 2, 2 to 3 and 3 to 2 (Fig. 2).

Bipartite property is important for considering random walks on graphs. We therefore generalize a lemma in paper [9]. Its proof seems similar. For convenience to read, we also present the proof here. For more references, see books [2,4].

Theorem 2.1. *G is bipartite if and only if $M_{k,n}(G)$ is bipartite.*

Proof. We use the classical result of König that a graph is bipartite if and only if all its cycles are even.

If G is not bipartite, then there is a cycle $C = v_1v_2\cdots v_mv_1$ of odd length in G. We look at the cycle in $M_{k,n}(G)$ given by

$$(v_1, v_1, \ldots, v_1)(v_1, \ldots, v_1, v_2)(v_1, \ldots, v_1, v_3)\cdots(v_1, \ldots, v_1, v_m)(v_1, \ldots, v_1, v_1).$$

Its length is also odd. Thus $M_{k,n}(G)$ is not bipartite.

If G is bipartite, then the set of vertices $V = V(G)$ can be written as $V_1 \cup V_2$, with $V_1 \cap V_2 = \emptyset$ and there is no edge between vertices both in V_1 or both in V_2. We try to bipart the set of vertices of $M_{k,n}(G)$. We know $V(M_{k,n}(G)) = V^{\times k}$. We write $V = V_1 + V_2$. Then

$$V^{\times k} = (V_1 \cup V_2)^{\times k} = V_1^k \cup V_1^{k-1}V_2 \cup V_1^{k-2}V_2^2 \cup \cdots \cup V_1V_2^{k-1} \cup V_2^k,$$

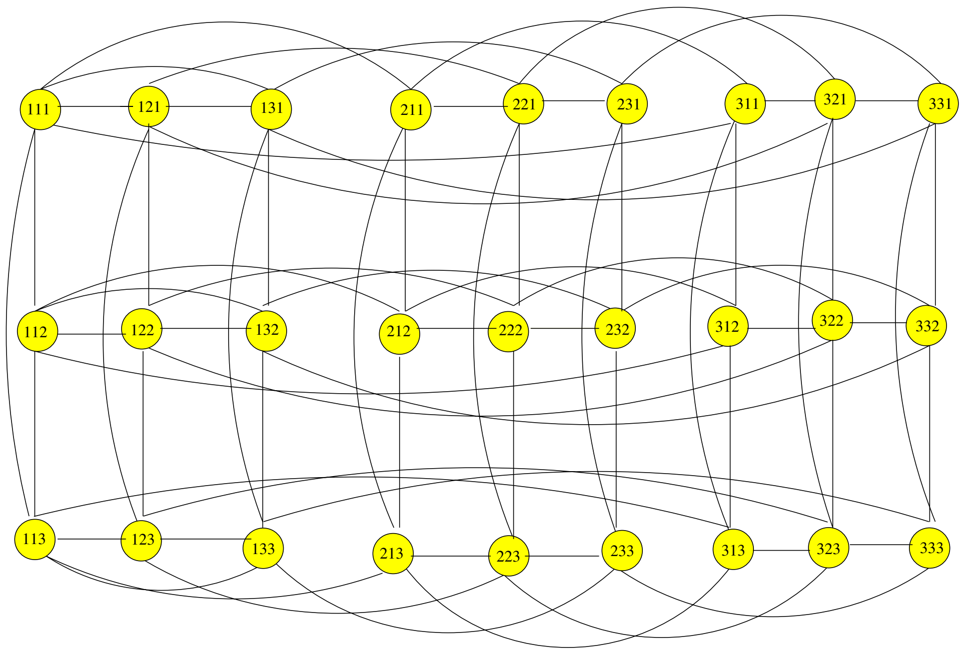

Fig. 2. The third tensor power $M_{3,3}(G)$ of G.

where $V_1^{k-r}V_2^r$ means we take $(k-r)$ vertices from V_1 and r vertices from V_2, regardless of order, to form a vertex of $M_{k,n}(G)$. Let

$$\overline{V_1} = V_1^k \cup V_1^{k-2}V_2^2 \cup V_1^{k-4}V_2^4 \cup \cdots,$$
$$\overline{V_2} = V_1^{k-1}V_2 \cup V_1^{k-3}V_2^3 \cup V_1^5 V_2^{k-5} \cup \cdots.$$

Then $\overline{V_1} \cup \overline{V_2} = V(M_{k,n}(G))$ and $\overline{V_1} \cap \overline{V_2} = \emptyset$. By the definition of $M_{k,n}(G)$, we cannot find an edge between any two vertices which are both in $\overline{V_1}$ or both in $\overline{V_2}$. $\square$

Remark 2.1. We could define the tensor products of any finite number of different graphs by a motivation from the tensor products of Markov processes in the next subsection. However, we leave it as a further topic.

2.2. The tensor products of Markov chains

The tensor products could be defined for any stochastic process in general. For our present purpose, we just define the tensor products for Markov chains including continuous time and discrete time cases.

Let $X_t^{(1)}, X_t^{(2)}, \ldots, X_t^{(k)}$ be Markov processes (Continuous time Markov chains with homogeneous transition probabilities here) on the state spaces $S^{(1)}, S^{(2)}, \ldots, S^{(k)}$, respectively. We define a new process Y_t on the state space $S^{(1)} \times S^{(2)} \times \cdots \times S^{(k)}$ with the transition probability given by

$$\begin{aligned}
&\Pr\{Y_{t+h} = (s_2) \mid Y_h = (s_1)\} \\
&\quad = \prod_{i=1}^{k} \Pr\{Y_{t+h}^{(i)} = s_2^{(i)} \mid Y_h^{(i)} = s_1^{(k)}\} \\
&\quad = \prod_{i=1}^{k} p^{(i)}_{s_1^{(i)} s_2^{(i)}}(t),
\end{aligned}$$

where $(s_j) = (s_j^{(1)}, s_j^{(2)}, \ldots, s_j^{(k)})$, $j = 1, 2$, and $p^{(i)}_{s_1^{(i)} s_2^{(i)}}(t)$ is the transition probability function of the Markov process $X_t^{(i)}$, $i = 1, 2, \ldots, k$.

We call Y_t the *tensor product* of Markov processes $X_t^{(i)}$, $i = 1, 2, \ldots, k$.

The next two statements are basic statements for the tensor products of Markov processes. We therefore give their proofs.

Lemma 2.1. *Y_t is a continuous time Markov chain.*

Proof. 1. By the definition of the tensor product Y_t its transition probability function

$$P_{(s_1)(s_2)}(t) = \prod_{i=1}^{k} p^{(i)}_{s_1^{(i)} s_2^{(i)}}(t) \geqslant 0,$$

since each term of the product is nonnegative.

2.

$$\sum_{(s_2)} P_{(s_1)(s_2)}(t) = \sum_{(s_2)} \prod_{i=1}^{k} p^{(i)}_{s_1^{(i)} s_2^{(i)}}(t) = \prod_{i=1}^{k} \sum_{s_2^{(i)} \in S^{(i)}} p^{(i)}_{s_1^{(i)} s_2^{(i)}}(t) = 1,$$

since each summation is one.

3. The Chapman–Kolmogorov equations,

$$\begin{aligned} P_{(s_1)(s_2)}(h+t) &= \prod_{i=1}^{k} p^{(i)}_{s_1^{(i)} s_2^{(i)}}(h+t) \\ &= \prod_{i=1}^{k} \sum_{s_3^{(i)} \in S^{(i)}} p^{(i)}_{s_1^{(i)} s_3^{(i)}}(h) p^{(i)}_{s_3^{(i)} s_2^{(i)}}(t) \\ &= \sum_{(s_3)} P_{(s_1)(s_3)}(h) P_{(s_3)(s_2)}(t), \end{aligned}$$

are satisfied.

4. We have the regularity,

$$\lim_{t \to 0^+} P_{(s_1)(s_2)}(t) = \lim_{t \to 0^+} \prod_{i=1}^{k} p^{(i)}_{s_1^{(i)} s_2^{(i)}}(t) = \begin{cases} 1 & \text{if } (s_1) = (s_2), \\ 0 & \text{otherwise,} \end{cases}$$

when $(s_1) = (s_2)$, each term of the product goes to one; when $(s_1) \neq (s_2)$, there is at least a term so that $s_1^{(r)} \neq s_2^{(r)}$, then $p^{(r)}_{s_1^{(r)} s_2^{(r)}}$ goes to zero.

Therefore, the definition of tensor products of Markov processes is well-defined. □

Theorem 2.2. *Let $q_{(s_1)(s_2)}$ be the infinitesimal generator of the continuous time Markov chain Y_t. Then*

$$q_{(s_1)(s_2)} = \begin{cases} q^{(i)}_{s_1^{(i)} s_2^{(i)}} & \textit{if } \exists \textit{ only one index } i \textit{ such that } s_1^{(i)} \neq s_2^{(i)}, \\ \sum_{i=1}^{k} q^{(i)}_{s_1^{(i)} s_2^{(i)}} & \textit{if } (s_1) = (s_2), \textit{ namely }, s_1^{(i)} = s_2^{(i)} \textit{ for all } i, \\ 0 & \textit{otherwise.} \end{cases}$$

where $q^{(i)}_{s_1^{(i)} s_2^{(i)}}$ is the infinitesimal generator of Markov process $X_t^{(i)}$, $i = 1, 2, \ldots, k$.

Proof. 1. If there exists only one index r such that $s_1^{(r)} \neq s_2^{(r)}$, then we have

$$\begin{aligned}
\lim_{t\to 0^+} \frac{\prod_{i=1}^k p^{(i)}_{s_1^{(i)} s_2^{(i)}}(t)}{t} &= \lim_{t\to 0^+} \frac{\prod_{i=1, i\neq r}^k p^{(i)}_{s_1^{(i)} s_2^{(i)}}(t) \times p^{(r)}_{s_1^{(r)} s_2^{(r)}}(t)}{t} \\
&= \prod_{i=1, i\neq r}^{k} p^{(i)}_{s_1^{(i)} s_2^{(i)}}(0) \lim_{t\to 0^+} \frac{p^{(r)}_{s_1^{(r)} s_2^{(r)}}(t)}{t} \\
&= 1 \times q^{(r)}_{s_1^{(r)} s_2^{(r)}} = q^{(r)}_{s_1^{(r)} s_2^{(r)}}.
\end{aligned}$$

2. If $(s_1) = (s_2)$, namely, $s_1^{(i)} = s_2^{(i)}$ for all i, then

$$\begin{aligned}
\lim_{t\to 0^+} \frac{\prod_{i=1}^k p^{(i)}_{s_1^{(i)} s_1^{(i)}}(t) - 1}{t} &= \lim_{t\to 0^+} \frac{[p^{(1)}_{s_1 s_1}(t) - 1]\prod_{i=2}^k p^{(i)}_{s_1^{(i)} s_1^{(i)}}(t) + \prod_{i=2}^k p^{(i)}_{s_1^{(i)} s_1^{(i)}}(t) - 1}{t} \\
&= q^{(1)}_{s_1^{(1)} s_1^{(1)}} + \lim_{t\to 0^+} \frac{[p^{(2)}_{s_1^{(2)} s_1^{(2)}}(t) - 1]\prod_{i=3}^k p^{(i)}_{s_1^{(i)} s_1^{(i)}}(t) + \prod_{i=3}^k p^{(i)}_{s_1^{(i)} s_1^{(i)}}(t) - 1}{t} \\
&= q^{(1)}_{s_1^{(1)} s_1^{(1)}} + q^{(2)}_{s_1^{(2)} s_1^{(2)}} + \cdots + \lim_{t\to 0^+} \frac{p^{(k)}_{s_1^{(k)} s_1^{(k)}}(t) - 1}{t} \\
&= \sum_{i=1}^{k} q^{(i)}_{s_1^{(i)} s_1^{(i)}}.
\end{aligned}$$

3. Except the cases of the above, there are at least two indices, say j and r, such that $s_1^{(j)} \neq s_2^{(j)}$ and $s_1^{(r)} \neq s_2^{(r)}$,

$$\begin{aligned}
\lim_{t\to 0^+} \frac{\prod_{i=1}^k p^{(i)}_{s_1^{(i)} s_2^{(i)}}(t)}{t} &= \prod_{i\neq r, i\neq j} p^{(i)}_{s_1^{(i)} s_2^{(i)}}(0) \times p^{(r)}_{s_1^{(r)} s_2^{(r)}}(0) \lim_{t\to 0^+} \frac{p^{(j)}_{s_1^{(j)} s_2^{(j)}}(t)}{t}. \\
&= 0.
\end{aligned}$$

Thus, we get the infinitesimal generator for the Markov process Y_t. □

Now, if we order the elements of the state space $S^{(1)} \times S^{(2)} \times \cdots \times S^{(n)}$ lexicographically, and let $P^{(i)}(t)$ be the probability transition matrix of $X_t^{(i)}$, $i = 1, 2, \ldots, k$, it is easy to see that the probability transition matrix $P(t)$ of Y_t is given by the tensor product

$$P^{(1)}(t) \otimes P^{(2)}(t) \otimes \cdots \otimes P^{(k)}(t).$$

This is why we call Y_t is a tensor product of Markov process $X_t^{(i)}$, $i = 1, 2, \ldots, k$. By Theorem 2.2, we also can see that the infinitesimal generator matrix of Y_t is given by

$$Q^{(1)} \otimes I \otimes \cdots \otimes I + I \otimes Q^{(2)} \otimes I \otimes \cdots \otimes I + \cdots + I \otimes \cdots \otimes I \otimes Q^{(k)},$$

where $Q^{(i)}$ is the infinitesimal generator matrix of $X_t^{(i)}$, $i = 1, 2, \ldots, k$. Thus, for convenience, we denote $Y_t = X_t^{(1)} \otimes X_t^{(2)} \otimes \cdots \otimes X_t^{(k)}$. We also have the following interesting statement by using these notations.

Corollary 2.1.

$$\begin{aligned}
P(t) &= P^{(1)}(t) \otimes P^{(2)}(t) \otimes \cdots \otimes P^{(k)}(t) \\
&= \exp((Q^{(1)} \otimes I \otimes \cdots \otimes I + I \otimes Q^{(2)} \otimes I \otimes \cdots \otimes I + \cdots + I \otimes \cdots \otimes I \otimes Q^{(k)})t).
\end{aligned}$$

Proof. For simplicity, we take factor number k to be 2 and denote $Q^{(1)}$ as Q, and $Q^{(2)}$ as $\overline{Q}$. We directly compute the results to verify our conceptual derivative.

$$\begin{aligned}
P(t) &= P^{(1)}(t) \otimes P^{(2)}(t) \\
&= \exp(Qt) \otimes \exp(\overline{Q}t) \\
&= \left(I + Qt + \frac{1}{2!}Q^2t^2 + \cdots\right) \otimes \left(I + \overline{Q}t + \frac{1}{2!}\overline{Q}^2t^2 + \cdots\right) \\
&= I \otimes I + (Q \otimes I + I \otimes \overline{Q})t + \left(\frac{1}{2}Q^2 \otimes I + \frac{1}{2}I \otimes \overline{Q}^2 + Q \otimes \overline{Q}\right)t^2 \\
&\quad + \left(\frac{1}{3!}Q^3 \otimes I + \frac{1}{3!}I \otimes \overline{Q}^3 + \frac{1}{2!}Q \otimes \overline{Q}^2 + \frac{1}{2!}Q^2 \otimes \overline{Q}\right)t^3 + \cdots \\
&= I + (Q \otimes I + I \otimes \overline{Q})t + \frac{1}{2!}(Q \otimes I + I \otimes \overline{Q})^2t^2 + \frac{1}{3!}(Q \otimes I + I \otimes \overline{Q})^3t^3 + \cdots \\
&= \exp((Q \otimes I + I \otimes \overline{Q})t).
\end{aligned}$$

Notice that if $X_t^{(1)}$ and $X_t^{(2)}$ have different numbers of states, the identity matrices in the above expressions have different sizes. □

2.3. Continuous time simple random walks on $M_{k,n}(G)$

In the paper [9], we introduced continuous time simple random walks (CTSRW) on graphs. For a given graph G, the CTSRW on G is defined by giving its infinitesimal generator as the negative Laplacian of G. We know that the jump chains of the CTSRWs on a graph are the simple random walks (SRW) on this graph. We could therefore estimate some interesting quantities about SRW by studying CTSRW. Surprisingly, by using the tensor powers of a graph, the k-coalescent random walk on the graph G turns out to be the jump chain of the CTSRW on the kth tensor power of G. Let us now denote Markov process CTSRW on $M_{k,n}(G)$ by Y_t, and Markov process CTSRW on G by X_t. We have the following basic statement.

Theorem 2.3. *The Markov process Y_t on the graph $M_{k,n}(G)$ is the kth tensor power of the Markov process X_t on the ground graph G. The jump chain of Y_t is k-coalescent random walk of G.*

Proof. Let us recall $Q = -L(G) = -D(G) + A(G) = (q_{ij})_{n\times n}$,

$$q_{ij} = \begin{cases} 1 & \text{if } ij \in E(G), \\ -d(i) & \text{if } i = j, \\ 0 & \text{otherwise,} \end{cases}$$

where $d(i)$ is the degree of the vertex i. Let $X_t \otimes X_t \otimes \cdots \otimes X_t = Z_t$ be the kth tensor power of the process X_t. Take two states for Z_t, (s_1) and (s_2). Then (s_i) actually is a sequence of vertices of G. We write $(s_1) = (i_1, i_2, \ldots, i_k)$ and $(s_2) = (j_1, j_2, \ldots, j_k)$. By Theorem 2.2 above, we have

$$\begin{aligned}
p'_{(s_1)(s_2)}(0) &= \begin{cases} q^{(r)}_{s_1^{(r)}s_2^{(r)}} & \text{if } \exists \text{ only one index } r \text{ such that } s_1^{(r)} \neq s_2^{(r)}, \\ \sum_{r=1}^k q^{(r)}_{s_1^{(r)}s_2^{(r)}} & \text{if } (s_1) = (s_2),\ \text{namely, } s_1^{(r)} = s_2^{(r)} \text{ for all } r, \\ 0 & \text{otherwise,} \end{cases} \\
&= \begin{cases} 1 & \text{if } \exists \text{ only one index } r \text{ such that } i_r \neq j_r,\ i_rj_r \in E(G), \\ -\sum_{r=1}^k d(i_r) & \text{if } i_r = j_r \text{ for all } r, \\ 0 & \text{otherwise.} \end{cases}
\end{aligned}$$

Now, we could identify (s_1) and (s_2) with the images of certain maps x and y, respectively. Then by the definition of $M_{k,n}(G)$, $xy \in E(M_{k,n}(G))$, if and only if $p'_{(s_1)(s_2)}(0) = 1$. As to the degree of x, we know that the neighbors of $x = (s_1)$ can only be $(r_1, i_2, \ldots, i_k)$, where r_1 must be a neighbor of i_1 in the ground graph G; $(i_1, r_2, \ldots, i_k)$, where

r_2 must be a neighbor of i_2 in the ground graph G; and so on, up to the last one $(i_1, i_2, \ldots, i_{k-1}, r_k)$, where r_k must be a neighbor of i_k in the ground graph G. Thus

$$d(x) = d(s_1) = \sum_{j=1}^{k} d(i_j).$$

This agrees with $p'_{(s_1)(s_1)}(0) = -\sum_{r=1}^{k} d(i_r)$. So, $Y_t = X_t \otimes X_t \otimes \cdots \otimes X_t = Z_t$.

The second conclusion is easy to see. □

Because of this theorem, we call graph $M_{k,n}(G)$ the kth tensor power of the graph G. We also note that the transition probability from x to y for Y_t is given by

$$P_{xy}(t) = \prod_{i=1}^{k} p_{x(i)y(i)}(t).$$

From the proof of Theorem 2.3, we know that for $x \in M_{k,n} = V(M_{k,n}(G))$, its degree in $M_{k,n}(G)$ is given by

$$d(x) = \sum_{r=1}^{k} d(x(r)).$$

We can compute the size of $M_{k,n}(G)$, i.e. the number of edges of $M_{k,n}(G)$ as

$$\begin{aligned} 2|E(M_{k,n}(G))| &= \sum_{x \in M_{k,n}} d(x) = \sum_{x \in M_{k,n}} \sum_{r=1}^{k} d(x(r)) = \sum_{r=1}^{k} \sum_{x \in M_{k,n}} d(x(r)) \\ &= \sum_{r=1}^{k} ((d(1) + d(2) + \cdots + d(k))n^{k-1}) \\ &= 2mkn^{k-1}. \end{aligned}$$

Thus, the size of $M_{k,n}(G)$ is mkn^{k-1}. It is clear that the order of $M_{k,n}(G)$ is n^k. Therefore, the frequency of $M_{k,n}(G)$ is $2mk/n$. The definition of the frequency is in paper [9]. We write these results as a corollary.

Corollary 2.2. *The kth tensor power of graph G with order n and size m has order and size*, *respectively*,

$$|V(M_{k,n}(G))| = n^k,$$

$$|E(M_{k,n}(G))| = mkn^{k-1}.$$

If G is not bipartite with order n and size m, then $M_{k,n}(G)$ is not bipartite. We could have the stationary distribution for the k-coalescent random walk on G. In terms of the SRW on graph $M_{k,n}(G)$, for each vertex x in $M_{k,n}$, the x-component of the stationary distribution is given by

$$\pi_x = \frac{d(x)}{2mkn^{k-1}} = \frac{\sum_{i=1}^{k} d(x(i))}{2mkn^{k-1}} = k^{-1}n^{1-k} \sum_{i=1}^{k} \frac{d(x(i))}{2m} = k^{-1}n^{1-k} \sum_{i=1}^{k} \pi^G_{x(i)},$$

where

$$\pi^G_{x(i)} = \frac{d(x(i))}{2m}$$

is the $x(i)$-component of the stationary distribution vector for SRW on G.

For a given map in $M_{k,n}$, the expected first return time for CTSRW on $M_{k,n}(G)$ is given by

$$h(x,x)=\frac{n^k}{d(x)}=\frac{n^k}{\sum_{i=1}^{k}d(x(i))}.$$

In particular, for the identity map Id, $d(Id)=d_1+d_2+\cdots+d_n=2m$. So

$$h(Id,Id)=\frac{n^k}{2m}.$$

For the jump chain SRW on $M_{k,n}(G)$, or k-coalescent random walk on G, we have

$$H(x,x)=f_{M_{k,n}(G)}h(x,x)=\frac{2mkn^{k-1}}{\sum_{i=1}^{k}d(x(i))},$$

where $f_{M_{k,n}(G)}=2mk/n$ is the frequency of $M_{k,n}(G)$. In particular,

$$H(Id,Id)=n^k.$$

Remark 2.2. When we talk about identity map above we require that the number of walkers is the same as the number of vertices of the graph.

2.4. *Coalescent times for k-coalescent random walk on G*

For CTSRW on $M_{k,n}(G)$, we are interested in calculating $h(x,c_i)$, the hitting time from x to c_i, where x represents the initial configuration of these k persons and c_i is the constant map to a vertex i of G. Once we know $h(x,c_i)$, we can use it to estimate $H(x,c_i)$ for SRW on $M_{k,n}(G)$, or equivalently, the expect number of steps k-coalescent random walk on G should take to have all persons first meet at the vertex i. That is the mean coalescent times for k-coalescent random walk on G. To compute this quantities, we need recall certain formula in paper [9] also books [3,8].

The mean hitting time for CTSRW on graph G with order n and size m from vertex i to j is given by the following integral:

$$h(i,j)=n\int_0^\infty (p_{jj}(t)-p_{ij}(t))\,\mathrm{d}t.$$

For continuous time Markov chains, particularly CTSRW on graphs, the "time-step inequality" states a relation between a Markov time T and steps N_T of the jump chains:

$$d_m E(T)\leqslant E(N_T)\leqslant d_M E(T).$$

Now, if the minimum and maximum degree of graph G are, respectively, d_m and d_M, then the minimum and maximum degree of graph $M_{k,n}(G)$ are, respectively, kd_m and kd_M. Therefore, we have

$$kd_m h(x,c_i)\leqslant H(x,c_i)\leqslant kd_M h(x,c_i).$$

Notice that when the graph G is regular, $H(x,c_i)$ is determined completely by $h(x,c_i)$: $H(x,c_i)=kd\cdot h(x,c_i)$.

Let x and y be two distinct vertices in $M_{k,n}(G)$, we consider the hitting time $h(x,y)$ of y from x in CTSRW. We have

$$\begin{aligned}h(x,y)&=n^k\int_0^\infty (P_{yy}(t)-P_{xy}(t))\,\mathrm{d}t\\&=n^k\int_0^\infty\left(\prod_{i=1}^{k}p_{y(i)y(i)}(t)-\prod_{i=1}^{k}p_{x(i)y(i)}(t)\right)\mathrm{d}t.\end{aligned}$$

For $y = c_i$, we have

$$h(x, c_i) = n^k \int_0^\infty \left(p_{ii}^k(t) - \prod_{i=1}^{k} p_{x(i)y(i)}(t) \right) \mathrm{d}t.$$

Thus, we get an estimation of the mean coalescent times $H(x, c_i)$ by $h(x, c_i)$ or the above integral.

It is interesting to look at a special case that in the beginning of the coalescent random walk there are r persons standing on each vertex. Let x_0 be the map represent the initial configuration of there rn persons. Then the integral becomes

$$h(x_0, c_i) = n^{rn} \int_0^\infty \left(p_{ii}^{rn}(t) - \prod_{j=1}^{n} p_{ji}^r(t) \right) \mathrm{d}t.$$

When r is one, that means, each vertex has one person in the beginning, we have

$$h(x_0, c_i) = n^n \int_0^\infty \left(p_{ii}^n(t) - \prod_{j=1}^{n} p_{ji}(t) \right) \mathrm{d}t.$$

To calculate this integral, we diagonalize the Laplacian of G. Write

$$U^{\mathrm{T}} Q U = \mathrm{diag}[-\lambda_1, -\lambda_2, \ldots, -\lambda_n],$$

where $U = (u_{ij})_{n\times n}$ is an orthogonal matrix. Then

$$p_{ij}(t) = \sum_{k=1}^{n} u_{ik} u_{jk} \mathrm{e}^{-\lambda_k t}.$$

Since

$$p_{ii}(t)^n = \left(\sum_{k=1}^{n} u_{ik}^2 \mathrm{e}^{-\lambda_k t} \right)^n = \sum_{1 \leqslant k_1, k_2, \ldots, k_n \leqslant n} u_{ik_1}^2 u_{ik_2}^2 \cdots u_{ik_n}^2 \mathrm{e}^{-(\lambda_{k_1} + \lambda_{k_2} + \cdots + \lambda_{k_n})t}$$

and

$$\prod_{k=1}^{n} p_{ki}(t) = \sum_{1 \leqslant k_1, k_2, \ldots, k_n \leqslant n} u_{1k_1} u_{ik_1} u_{2k_2} u_{ik_2} \cdots u_{nk_n} u_{ik_n} \mathrm{e}^{-(\lambda_{k_1} + \lambda_{k_2} + \cdots + \lambda_{k_n})t},$$

we get

$$h(Id, c_i) = n^n \sum_{1 \leqslant k_1, k_2, \ldots, k_n \leqslant n} \frac{u_{ik_1}^2 u_{ik_2}^2 \cdots u_{ik_n}^2 - u_{1k_1} u_{ik_1} u_{2k_2} u_{ik_2} \cdots u_{nk_n} u_{ik_n}}{\lambda_{k_1} + \lambda_{k_2} + \cdots + \lambda_{k_n}}.$$

Example. Let G be the triangle graph. It is regular with $n = 3$ and $d = 2$. The matrix Q and U are given below

$$Q = \begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix} \quad \text{and} \quad U = \begin{pmatrix} -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ 0 & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \end{pmatrix}.$$

We have $U^{\mathrm{T}} Q U = \mathrm{diag}[-3, -3, 0]$. Since $\lambda_3 = 0$, when calculating $h(Id, c_i)$, we should drop the term $(k_1, k_2, k_3) = (3, 3, 3)$. Notice that the numerator of this term in $h(Id, c_i)$ is also zero, so it is fine to drop this term. We have

$$h(Id, c_1) = 3^3 \cdot \frac{31}{162} = \frac{31}{6}.$$

So

$$H(Id, c_1) = 3 \cdot 2 \cdot \frac{31}{6} = 31.$$

Thus, for our coalescent random walk on the triangle graph, it takes 31 steps on average for three persons to meet at any specified vertex, given that they all start at different vertices.

For the square graph with $n = 4$ and $d = 2$, a similar calculation shows

$$h(Id, c_1) = 4^4 \cdot \frac{167}{1120} = \frac{1336}{35}$$

and

$$H(Id, c_1) = 8 \cdot \frac{1336}{35} \approx 305.371.$$

Thus, for our coalescent random walk on the square graph, it takes about 305 steps on average for four persons to meet at any specified vertex, given that they all start at different vertices.

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