

Random line graphs and a linear law for assortativity

Dajie Liu,^{*} Stojan Trajanovski, and Piet Van Mieghem

Delft University of Technology, P.O Box 5031, NL-2600 GA Delft, The Netherlands

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For a fixed number N of nodes, the number of links L in the line graph $H(N, L)$ can only appear in consecutive intervals, called a band of L . We prove that some consecutive integers can never represent the number of links L in $H(N, L)$, and they are called a bandgap of L . We give the exact expressions of bands and bandgaps of L . We propose a model which can randomly generate simple graphs which are line graphs of other simple graphs. The essence of our model is to merge step by step a pair of nodes in cliques, which we use to construct line graphs. Obeying necessary rules to ensure that the resulting graphs are line graphs, two nodes to be merged are randomly chosen at each step. If the cliques are all of the same size, the assortativity of the line graphs in each step are close to 0, and the assortativity of the corresponding root graphs increases linearly from -1 to 0 with the steps of the nodal merging process. If we dope the constructing elements of the line graphs—the cliques of the same size—with a relatively smaller number of cliques of different size, the characteristics of the assortativity of the line graphs is completely altered. We also generate line graphs with the cliques whose sizes follow a binomial distribution. The corresponding root graphs, with binomial degree distributions, zero assortativity, and semicircle eigenvalue distributions, are equivalent to Erdős-Rényi random graphs.

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I. INTRODUCTION

A simple graph [1] with N nodes and L links is denoted by $G(N, L)$. The line graph H of a simple graph G is a graph in which every node corresponds to a link in G and two nodes in H are adjacent if and only if their corresponding links in G share a node. The graph G is called the root graph or the original graph of H . The number N_H of nodes in H equals the number L of links in G . Whitney's Theorem [2,3] states that, if connected graphs G_1 and G_2 have isomorphic line graphs, G_1 and G_2 themselves must be isomorphic unless one is K_3 and the other is $K_{1,3}$. Cvetković *et al.* [4] surveyed the literature on line graphs.

Line graphs can model many real-world networks. For instance, a network of tennis players is formed when we connect two players who have played in the same game and a network of tennis games is a graph where two games are linked if the same competitors have played in both of them. The network of tennis games is the line graph of the network of tennis players [5]. In metabolisms, the chemical reaction network in which the nodes are the reactions and two nodes are linked if they have the same chemical compound, is the line graph of the chemical compound network in which the nodes are the compounds and two nodes are linked if they are involved in the same chemical reaction [6,7]. Line graphs can also model social networks as they are highly clustered and assortative [5,6,8,9]. Moreover, line graphs have been used in detecting and modeling the overlapping community structure in social networks [10–12].

Despite the significance of line graphs in the field of graph theory and complex networks, a model to generate random line graphs is still lacking. In this paper, we propose a model to randomly generate line graphs with a prescribed number of nodes and number of links. Before introducing the model, we discuss some preliminaries and various properties of random

line graphs. Especially, we show that, given the fixed number of nodes, the number L of links in line graphs possesses forbidden gaps in the set \mathbb{N} of integers. Without generating the root graphs first, our model is capable of generating line graphs with specific link density and assortativity. Our model also enables us to generate a group of root graphs whose assortativity coefficient strictly follows a linear law. Our model constructs line graphs by merging step by step a pair of nodes in a group of separate cliques. The nodal merging at each step must be implemented following certain rules which ensure that the constructed graphs are line graphs. Two nodes, which are merged at each step, are randomly chosen. Given the cliques of the same size, the assortativity [13,14] of the line graphs in each step is close to 0, and the assortativity of the corresponding root graphs has a linear relationship with the steps of the merging process. If a relatively smaller number of cliques of different size are added to the majority cliques of the same size, the characteristics of the assortativity of the line graphs become largely different. The line graphs are also constructed with the cliques whose sizes follow a binomial distribution. The corresponding root graphs appear equivalent to Erdős-Rényi random graphs with binomial degree distributions, zero assortativity, and semicircle eigenvalue distributions.

The remainder of the paper is organized as follows. Theoretical preliminaries for constructions line graphs are given in Sec. II. The random line graph model is presented in Sec. III. Section IV provides insights of the topological properties of the line graphs during the merging process. We conclude in Sec. V.

II. THEORETICAL PRELIMINARIES

A. Formation of line graphs

All the line graphs are simple graphs, but not all simple graphs are line graphs. Krausz's Theorem gives the criterion to determine whether a simple graph is a line graph. According

^{*}d.liu@tudelft.nl; liudajie.tudelft@gmail.com

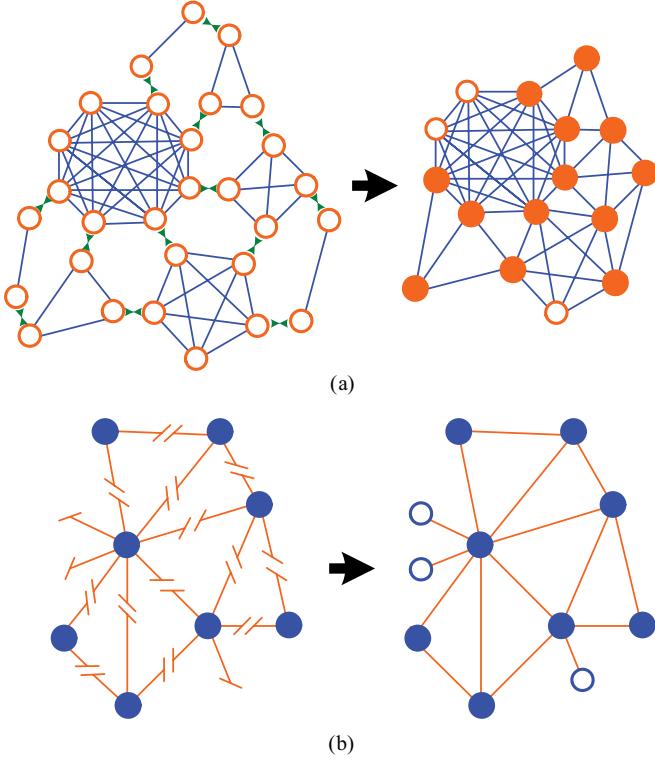


FIG. 1. (Color online) (a) The example of constructing a line graph by merging the half nodes of cliques, and (b) the example of constructing a simple graph by the configuration model. The circles and disks denote the half nodes and nodes respectively. The lines with slash ending and the normal lines denote the half links and links, respectively.

to Krausz's Theorem [15–17], line graphs can be partitioned into cliques which may have nodes in common.

Theorem 1 (Krausz). A graph is a line graph if and only if its sets of links can be partitioned into nontrivial cliques such that (i) two cliques have at most one node in common and (ii) each belongs to at most two cliques.

Our method to construct line graphs consists of combining separate cliques, obeying certain rules to ensure that the resulting graphs satisfy Krausz's Theorem. Before explaining the details of our method, we introduce the concept of "half node."

Definition 2. A half node is the comprising part of a node and two merged half nodes form a node. A half node is the map of a half link (stub) in the configuration model [18,19].

In order to construct a graph of size N where node j has degree d_j with the configuration model [18,19], we need N separate nodes where d_j half links (also called stubs by some authors) are incident to node j . Two combined half links form a link. Every half link has to be combined with another half link. Inspired by the configuration model for the root graphs, we develop a method to construct the line graphs. We need separate cliques consisting of fully connected half nodes, as shown in Fig. 1(a). A half node is the map of a half link in the configuration model. Two merged half nodes form a node in the line graph. Like a node, a half node is an abstract concept without any quantity. When two half nodes merge into a new node, the links incident to either of the two half nodes are

attached to the new node, and the link (if any) between the two half nodes is deleted, as shown in Fig. 1(a).

To construct a line graph, every half node has to be merged with another half node. We randomly choose and merge a pair of half nodes, under the constraints that (1) *the two half nodes belong to different cliques and (2) the cliques, to which the two half nodes belong, have no nodes in common*. Once merged, two half nodes form a node of the line graph. The construction continues until all half nodes are merged. The rules assure that the graphs constructed by merging the half nodes of cliques satisfy the criteria in Theorem 1 and thus are line graphs.

The "elements" for construction of line graphs, which are the cliques of half nodes, can be regarded as the atoms, hence the formation of line graphs is analogous to the formation of a molecule. The merging of two half nodes is analogous to the formation of the chemical bond. Interestingly, we never see more than one chemical bond between two atoms in a molecule or a chemical bond formed with a single atom, which conforms to our rules of forming line graphs. Figure 1(a) depicts a line graph constructed from a clique of K_8 , a clique of K_6 , a clique of K_5 , two cliques of K_4 , two cliques of K_3 , four cliques of K_2 , and three cliques of K_1 . The root graph of the line graph (a) is shown in Fig. 1(b).

B. The bandgaps of the number of links L in line graph $H(N,L)$

In this section, we investigate which integers can occur as the number of links L in the line graph $H(N,L)$.

The number of links L in the line graph $H(N,L)$ with N nodes satisfies $L \leq L_{\max} = \binom{N}{2}$, and $L = \binom{N}{2}$ only if the line graph H is a complete graph K_N . The principal clique in a line graph $H(N,L)$ is defined by the largest clique in H .

Lemma 3. Suppose that the principal clique K_{N-k+1} , where $2 \leq k \leq \lfloor \frac{N+1}{2} \rfloor$, in the line graph $H(N,L)$ consists of nodes n_k, n_{k+1}, \dots, n_N , as shown in Fig. 2(a). The minimum number

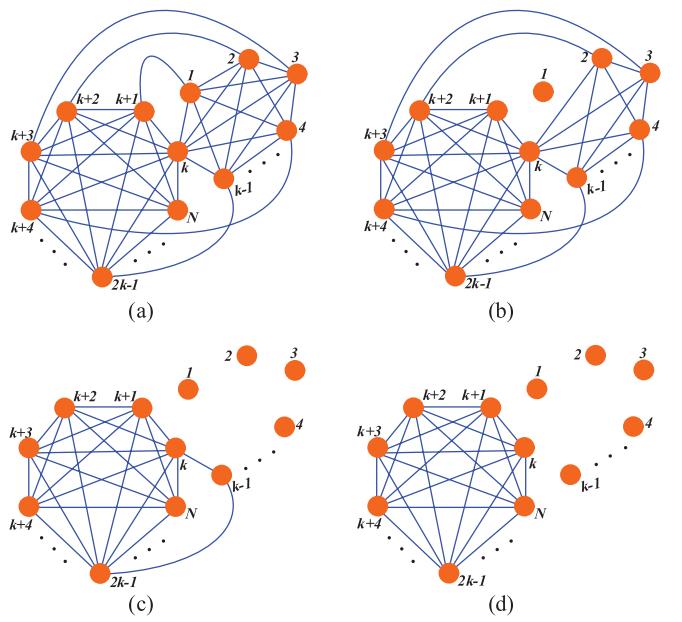


FIG. 2. (Color online) The configuration of $H(N,L)$ for (a) W_k ; (b) W_{k-1} ; (c) W_2 ; (d) W_1 . The labels of the nodes locate by the side of them.

of links in $H(N,L)$ is $L = \binom{N-k+1}{2}$, and the maximum number of links in $H(N,L)$ is $L = \binom{N-k+1}{2} + \binom{k}{2} + k - 1$.

Proof. The number of links in the principal clique K_{N-k+1} is $\binom{N-k+1}{2}$. When n_1, n_2, \dots, n_{k-1} are isolated nodes, the number of links in H is minimal and equals $L = \binom{N-k+1}{2}$. According to Theorem 1, each node of n_1, n_2, \dots, n_{k-1} belongs to at most two cliques, each of which contains a node which also belongs to the principal clique. For instance, node n_1 in Fig. 2(a) belongs to a clique K_2 , containing node n_{k+1} , and a clique K_k , containing node n_k . Hence, each node of n_1, n_2, \dots, n_{k-1} can have at most two links connecting itself and two nodes of the principal clique, contributing at most in total $2k-2$ links to the line graph. There are at most $\binom{k-1}{2}$ links to fully connect the nodes n_1, n_2, \dots, n_{k-1} , thus, the maximum number of links in $H(N,L)$ is $L = \binom{N-k+1}{2} + \binom{k-1}{2} + 2k-2 = \binom{N-k+1}{2} + \binom{k}{2} + k - 1$.

Theorem 4. Let $V_1 = \{\binom{N}{2}\}$. For $2 \leq k \leq \lfloor \frac{N+1}{2} \rfloor$, let

$V_k = \{\binom{N-k+1}{2}, \binom{N-k+1}{2} + 1, \dots, \binom{N-k+1}{2} + \binom{k}{2} + k - 1\}$. Then L is the number of links in the line graph $H(N,L)$, if and only if L is a integer and

$$L \in \left(\bigcup_{k=1}^{\lfloor \frac{N+1}{2} \rfloor} V_k \right) \cup \left\{ 0, 1, \dots, \left(\binom{\lfloor \frac{N+1}{2} \rfloor}{2} \right) + \left\lfloor \frac{N+1}{2} \right\rfloor - 1 \right\}.$$

Proof. See Appendix A. ■

Corollary 5. If $\lfloor \frac{-3+\sqrt{17+8N}}{2} \rfloor \leq k \leq \lfloor \frac{N+1}{2} \rfloor$, there is no gap between V_k and V_{k-1} .

Proof. When the largest element of V_k plus 1 is not smaller than the smallest element of V_{k-1} , there is no gap between V_k and V_{k-1} .

$$\binom{N-k+1}{2} + \binom{k}{2} + k - 1 + 1 \geq \binom{N-(k-1)+1}{2},$$

which is equivalent to

$$k^2 + 3k - (2N + 2) \geq 0,$$

from which Corollary 5 follows. ■

The width ΔV_k of the k th band V_k of L for the line graph $H(N,L)$, defined by the number of integers in the band, equals

$$\begin{aligned} \Delta V_k &= \binom{N-k+1}{2} + \binom{k}{2} + k - 1 - \binom{N-k+1}{2} + 1 \\ &= \binom{k}{2} + k, \end{aligned} \quad (1)$$

where $2 \leq k \leq \lfloor \frac{N+1}{2} \rfloor$. The k th bandgap Ψ_k of L for the line graph $H(N,L)$ is

$$\Psi_k = \left\{ \Gamma, \Gamma + 1, \Gamma + 2, \dots, \binom{N-k+1}{2} - 1 \right\},$$

where $\Gamma = \binom{N-k}{2} + \binom{k+1}{2} + k + 1$ and $1 \leq k \leq \lfloor \frac{N+1}{2} \rfloor - 1$. The width $\Delta \Psi_k$ of the k th bandgap of L is defined by the number of integers in the bandgap,

$$\begin{aligned} \Delta \Psi_k &= \binom{N-k+1}{2} - 1 - \left(\binom{N-k}{2} + \binom{k+1}{2} + k \right) \\ &= N - \frac{k^2 + 5k}{2} - 1. \end{aligned} \quad (2)$$

When $\Delta \Psi_k = N - \frac{k^2 + 5k}{2} - 1 < 1$, or equivalently when $1 \leq k \leq \lfloor (\sqrt{9+8N} - 5)/2 \rfloor$, the k th bandgap of L vanishes. Figure 3 shows that there are no bandgaps when $N \leq 4$. We also observe that, for those N making $(\sqrt{9+8N} - 5)/2$ an integer, the width of the bandgap $\Psi_{\lfloor (\sqrt{9+8N} - 5)/2 \rfloor}$ is 1. As shown in Fig. 3, when $N = 5, 9, 14$, we have $(\sqrt{9+8N} - 5)/2 = 1, 2, 3$, and the width of the last bandgap is 1. The line graphs, whose number L of links falls into the band gaps, do not exist. If we define the energy of a line graph by the number of links in that line graph, the bands and the bandgaps of L can be regarded as energy bands and energy bandgaps of the line graph.

III. A RANDOM LINE GRAPH MODEL

Based on the theory introduced in Sec. II, we propose a model which generates random line graphs. In the description of the model, we do not distinguish half nodes and nodes. The model starts with separate cliques and merges two randomly

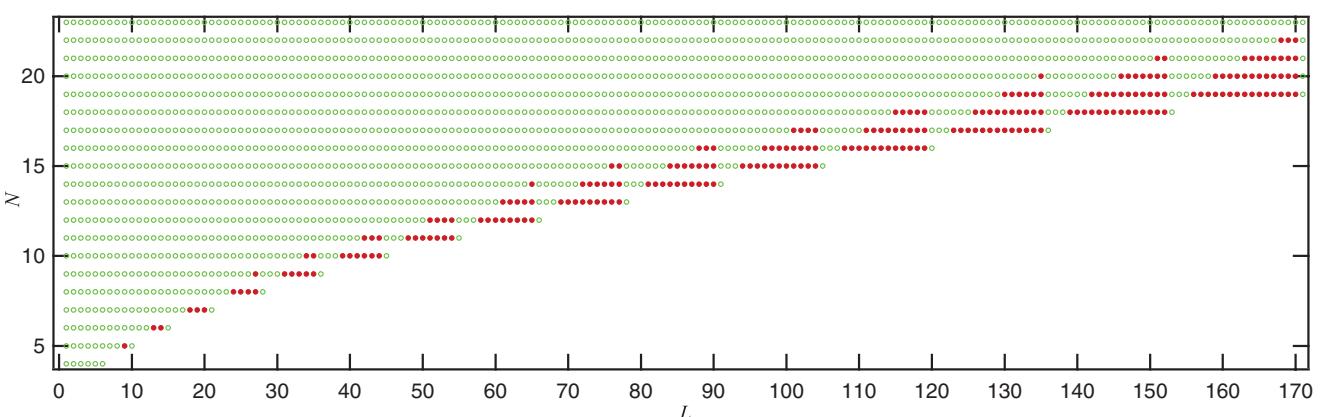


FIG. 3. (Color online) The bandgaps of L for $N = 4, 5, \dots, 14$. The solid dots denote the forbidden integers, while the hollow circles denote the possible integers as the number of links L .

Algorithm 1: $H \leftarrow \text{RandomLineGraph}(s)$

1. Construct a graph H consisting of the separate cliques whose sizes are the integers in the vector $s = [s_1 \ s_2 \ \cdots \ s_C]^T$, and all the integers are larger than 1.
 2. $\mathcal{N}_m \leftarrow$ the set of nodes in H
 3. **Repeat**
 4. Randomly choose two nodes j_1, j_2 in \mathcal{N}_m , which satisfy $l_{j_1, j_2} > 2$
 5. Merge j_1 and j_2
 6. $\mathcal{N}_m \leftarrow \mathcal{N}_m \setminus \{j_1, j_2\}$
 7. $N \leftarrow N - 1$
 8. **Until** no nodes j_1, j_2 in \mathcal{N}_m satisfying $l_{j_1, j_2} > 2$
-

selected nodes at each step. The merging of two nodes j_1 and j_2 in $H(N, L)$ is defined by deleting node j_2 and the link connecting nodes j_1 and j_2 , and attaching the links, which are only incident to j_2 , to j_1 . The model is presented in Algorithm 1. Theorem 6 guarantees that the graphs constructed by Algorithm 1 are line graphs. In Theorem 6, l_{j_1, j_2} denotes the length of the shortest path between node j_1 and node j_2 .

Theorem 6. The line graph H consisting of separate cliques remains a line graph after the merging of any pair of nodes j_1 and j_2 satisfying $l_{j_1, j_2} > 2$.

Proof. The randomly chosen nodes j_1 and j_2 do not belong to the same clique, otherwise $l_{j_1, j_2} = 1$, contradicting with the fact $l_{j_1, j_2} > 2$. The two cliques, to which j_1 and j_2 belong, respectively, do not share a node, otherwise there would be a hop $j_1 \sim j_0 \sim j_2$, where j_0 is the node shared by them, and thus $l_{j_1, j_2} = 2$, which contradicts with $l_{j_1, j_2} > 2$. Therefore, the nodes j_1 and j_2 are from two different cliques which have no nodes in common. After merging of nodes j_1 and j_2 , the graph H satisfies Theorem 1, hence, it remains a line graph. ■

A sequence of integers $s = [s_1 \ s_2 \ \cdots \ s_C]^T$ are designated as the sizes of the cliques (line 1). All the integers are larger than one, $s_j \geq 2, j = 1, 2, \dots, C$. These numbers are actually the degrees of the nodes in the root graph, that correspond to the cliques in the line graph. A graph $H(N, L)$ consisting of the separate cliques whose sizes are the given sequence of numbers is constructed (line 1). The number of nodes N equals $\sum_{j=1}^C s_j$, and the number of links L equals $\sum_{j=1}^C \binom{s_j}{2}$. Initially each of the nodes in H belongs to only one clique, and hence, are expansive nodes. The set of all expansive nodes in H is denoted by \mathcal{N}_m , which before the first merging is the set of nodes in H (line 2). Two nodes j_1 and j_2 are uniformly [20] chosen in \mathcal{N}_m , between which the shortest path length $l_{j_1, j_2} > 2$ (line 4). Nodes j_1 and j_2 are merged (line 5), and removed from \mathcal{N}_m (line 6), and the number of nodes N in the line graph H decreases by 1 (line 7). Lines 4–7 are repeated until there are no nodes j_1, j_2 in \mathcal{N}_m satisfying $l_{j_1, j_2} > 2$ (lines 3 and 8). Theorem 6 ensures that H remains a line graph after each execution of lines 4–7.

Theorem 7. The maximal number η of mergings that are performed in Algorithm 1 satisfies $\eta \leq \min(\lfloor \frac{1}{2} \sum_{j=1}^C s_j \rfloor, \binom{C}{2})$.

Proof. In a line graph, each node belongs to at most two cliques, therefore, the maximal number $\eta \leq \frac{1}{2} \sum_{j=1}^C s_j$

if $\sum_{j=1}^C s_j$ is an even number, and the maximal number $\eta \leq \frac{1}{2} \sum_{j=1}^C s_j - \frac{1}{2}$ if $\sum_{j=1}^C s_j$ is an odd number. Hence, $\eta \leq \lfloor \frac{1}{2} \sum_{j=1}^C s_j \rfloor$. In a line graph, each pair of cliques can have at most one node in common, therefore, the maximal number of mergings is also bounded by $\binom{C}{2}$. Hence, the maximal number of mergings $\eta \leq \min(\lfloor \frac{1}{2} \sum_{j=1}^C s_j \rfloor, \binom{C}{2})$. ■

IV. THE ASSORTATIVITY OF LINE GRAPH H AND CORRESPONDING ROOT GRAPH DURING THE MERGING PROCESS

In the susceptible-infectious-susceptible (SIS) model [21,22] for network epidemics, the network is infected in the steady state if the effective infection rate τ is larger than the epidemic threshold τ_c , and the network is virus free in the steady state when $\tau < \tau_c$. By the N -intertwined mean-field approximation (NIMFA) [21], the exact SIS epidemic threshold τ_c is lower bounded,

$$\tau_c \geq \tau_c^{(1)} = \frac{1}{\lambda_1(A)},$$

where $\lambda_1(A)$ is the largest eigenvalue of the adjacency matrix A of a network and is often called the spectral radius of the network. When the lower bound $\tau_c^{(1)}$ for the epidemic threshold is increased in a network, we are always sure that the real epidemic threshold (which is in most cases difficult to compute) is on the safe side. The largest eigenvalue $\lambda_1(A)$ also plays an important role in the phase-transition threshold of a network of coupled oscillators [22,23].

The largest eigenvalue $\lambda_1(A)$ is closely related to the assortativity coefficient ρ_D : $\lambda_1(A)$ increases with ρ_D . The minimum and maximum assortativity of a graph is computed in [24]. Several lower bounds for $\lambda_1(A)$ are given in [25]. The assortativity coefficient ρ_D can be increased or decreased by the degree-preserving rewiring [25]. However, $\rho_D(t)$ as a function of the step t of rewiring is unknown. Apart from altering the epidemic threshold by changing the graph's assortativity, link and node removals are another way to modify the largest eigenvalue of networks [22]. In this section, we show that the assortativity coefficient $\rho_D(G, t)$ of the root graph G of the line graph at the step t is a linear function of t in the nodal merging process of the random line graph model described in Algorithm 1.

A. Random line graphs with cliques of the same size $s_j = S$ for $j = 1, 2, \dots, C$

We construct line graphs with the random line graph model in Algorithm 1. We take 50 cliques of the same size S , and randomly choose and merge two nodes with shortest path larger than 2 until there are no such pair of nodes. After each step t of merging two nodes, the assortativity coefficient ρ_D of the line graph H and the corresponding root graph G are computed. The plots of $\rho_D(H, t)$ and $\rho_D(G, t)$ with $S = 2, 3, 4, 5, 6, 7$ are shown, respectively, in Fig. 4. The numerical results show that the assortativity of the line graph, $\rho_D(H, t)$, is close to 0 for $S = 3, 4, 5, 6, 7$, and the assortativity of the line

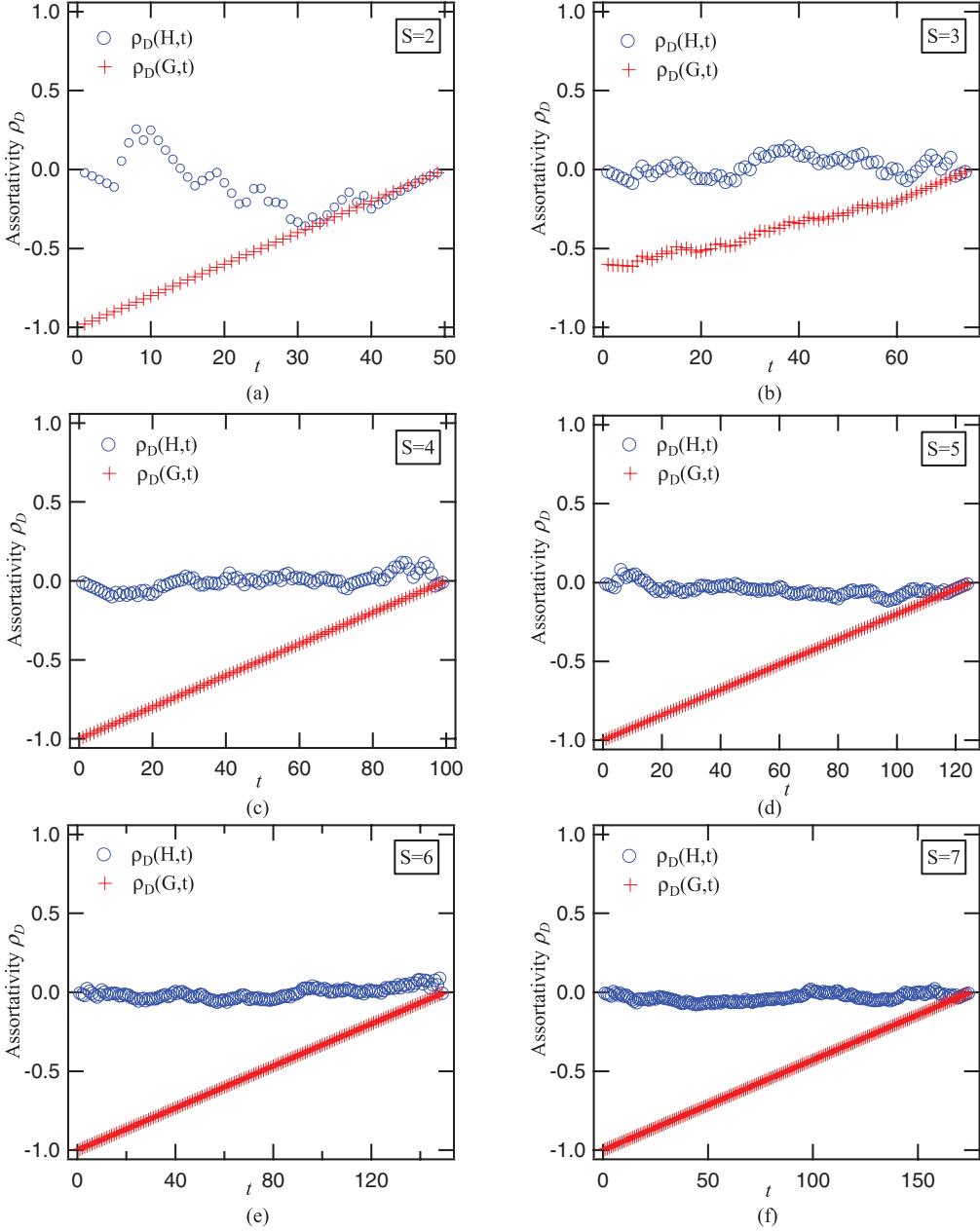


FIG. 4. (Color online) Using the line graph model, we construct line graphs with 50 cliques of the same size S . The assortativity coefficient of the line graphs and the corresponding root graphs are drawn as functions of the steps t of the nodal merging process. The root graphs of the line graphs are computed by ILIGRA, the inverse line graph construction algorithm [26]. One can also use other algorithms [27–29] to compute the root graphs.

graph, $\rho_D(G,t)$, increases linear with t for $S = 2, 4, 5, 6, 7$. We give the analytical analysis below.

1. Assortativity of line graphs

In the random line graph model, there are initially C separate cliques of size S . Hence, $H(N,L)$ has $N = CS$ nodes with degree $d_j = S - 1$ for $j = 1, 2, \dots, N$. The number of links $L = C\binom{S}{2}$ is constant in the process of consecutive merging of two nodes. The assortativity coefficient ρ_D of a

graph is expressed [see Eq. (7) in [25]] as

$$\rho_D = 1 - \frac{\sum_{i \sim j} (d_i - d_j)^2}{\sum_{i=1}^N d_i^3 - \frac{1}{2L} (\sum_{i=1}^N d_i^2)^2}, \quad (3)$$

where $\sum_{i \sim j}$ denotes the sum over all adjacent pairs of nodes. For simplicity, we denote the numerator by $A = \sum_{i \sim j} (d_i - d_j)^2$ and the denominator by $B = \sum_{i=1}^N d_i^3 - \frac{1}{2L} (\sum_{i=1}^N d_i^2)^2$, hence $\rho_D = 1 - \frac{A}{B}$.

When $t = 1$, we have 1 node with degree $2(S - 1)$ and $CS - 2$ nodes with degree $S - 1$. Furthermore, when $t = 2$,

we have 2 nodes with degree $2(S - 1)$ and $CS - 4$ with degree $S - 1$. After t steps of merging, there are t nodes with degree $2(S - 1)$ and $CS - 2t$ nodes with degree $S - 1$, and $N = CS - t$. The denominator B in (3) for $\rho_D(H,t)$ is

$$\begin{aligned} B &= \sum_{i=1}^N d_i^3 - \frac{1}{2L} \left(\sum_{i=1}^N d_i^2 \right)^2 \\ &= 8t(S - 1)^3 + (CS - 2t)(S - 1)^3 \\ &\quad - \frac{1}{CS(S - 1)} (4t(S - 1)^2 + (CS - 2t)(S - 1)^2)^2 \\ &= \frac{(S - 1)^3 2t}{CS} (CS - 2t). \end{aligned} \quad (4)$$

For the numerator A in (3), we consider the following cases:

(1) When $t \leq \frac{C}{2}$, each of the t nodes with degree $2(S - 1)$, is adjacent with on average $2(S - 1)$ nodes with degree $S - 1$. There is no degree difference among t nodes with degree $2(S - 1)$, and no degree difference among $2(S - 1)$ nodes with degree $S - 1$. Hence,

$$A = \sum_{i \sim j} (d_i - d_j)^2 \approx 2t(S - 1)^3. \quad (5)$$

Substituting (4) and (5) into (3) yields

$$\rho_D(H,t) \approx 1 - \frac{2t(S - 1)^3}{\frac{(S-1)^3 2t}{CS} (CS - 2t)} = \frac{\frac{2t}{CS}}{\frac{2t}{CS} - 1}.$$

Since $t \leq \frac{C}{2}$, the inequality $\frac{2t}{CS} \leq \frac{1}{S}$ holds. When S is large, $\rho_D(H,t)$ tends to 0.

(2) When $t \approx C$, each of the t nodes with degree $2(S - 1)$, is adjacent with on average $2(S - 2)$ nodes with degree $(S - 1)$. We have

$$A = \sum_{i \sim j} (d_i - d_j)^2 \approx 2t(S - 2)(S - 1)^2.$$

Hence,

$$\rho_D(H,t) \approx 1 - \frac{(S - 2)}{(S - 1) \left(1 - \frac{2t}{CS} \right)}.$$

The condition $t \approx C$ leads to $\frac{2t}{CS} \approx \frac{2}{S}$. The assortativity $\rho_D(H,t)$ is close to 0 for large S .

(3) When $t \approx \frac{N}{2} = \frac{CS}{2}$, most of nodes in H have degree $2(S - 1)$, therefore, $\sum_{i \sim j} (d_i - d_j)^2$ is close to 0. Since $t \approx \frac{CS}{2}$, the denominator is also close to 0, hence $\rho_D(H,t)$ is close to 0.

Results obtained in cases 1, 2, and 3 correspond to the simulation results for $\rho_D(H,t)$ in Fig. 4. A node with degree $2(S - 1)$ is adjacent with on average $2(S - 1)$ nodes of degree $S - 1$ when $t \leq \frac{C}{2}$, and with on average $2(S - 2)$ nodes of degree $S - 1$ when $t \approx C$. Hence, we deduce that a node with degree $2(S - 1)$ is adjacent with on average $2(S - \frac{2C}{t})$ nodes of degree $S - 1$ after t steps of mergings. This provides another method to estimate the numerator in (3):

$$\begin{aligned} A &= \sum_{i \sim j} (d_i - d_j)^2 \approx t \cdot 2 \left(S - \frac{2t}{C} \right) (2(S - 1) - (S - 1))^2 \\ &= \frac{2t}{C} (CS - 2t)(S - 1)^3. \end{aligned} \quad (6)$$

Hence, the assortativity of the line graph H is approximated by

$$\rho_D(H,t) \approx 1 - \frac{\frac{2t}{C} (CS - 2t)(S - 1)^2}{\frac{(S-1)^3 2t}{CS} (CS - 2t)} = \frac{1}{S}.$$

This approximate result also agrees well with the simulations in Fig. 4: When S increases, ρ_D becomes closer to 0.

If the selection procedure in line 4 of Algorithm 1 is not uniformly at random, the expression (4) of denominator B will be still valid, since the cliques are all of the same size S . However, the numerator A could be very different depending on how two nodes are selected at each step. The assortativity of the line graphs may not be close to 0. In case 1, $t \leq \frac{C}{2}$, and case 2, $t \approx C$, the line graphs could be very assortative or disassortative. In case 3, $t \approx \frac{N}{2} = \frac{CS}{2}$, it is still true that most of the nodes in H have been merged, and most nodes have degree $2(S - 1)$. Hence, we have the numerator $A = \sum_{i \sim j} (d_i - d_j)^2 \approx 0$ and the assortativity coefficient $\rho_D \approx 0$.

2. Assortativity of root graphs

When $t = 0$, H consists of C separate cliques with S nodes, and the corresponding root graph $G(N_G, L_G)$ consists of C separate complete bipartite graph $K_{1,S}$, which are star graphs. Hence, $\rho_D(G,t) = -1$ [see Eq.(9) in [25]]. Each star graph $K_{1,S}$ has 1 node with degree S , and S nodes with degrees 1. Hence, $N_G = C(S + 1)$ and $L_G = CS$, and there are in total C nodes with degrees S , and CS nodes with degree 1. The root graph in the step t consists of interconnected star graphs (Fig. 5), whose structure models the power law or scale-free structure of general complex networks well.

Theorem 8. In the merging step t in the Algorithm 1, the assortativity coefficient of the root graph G is a linear function

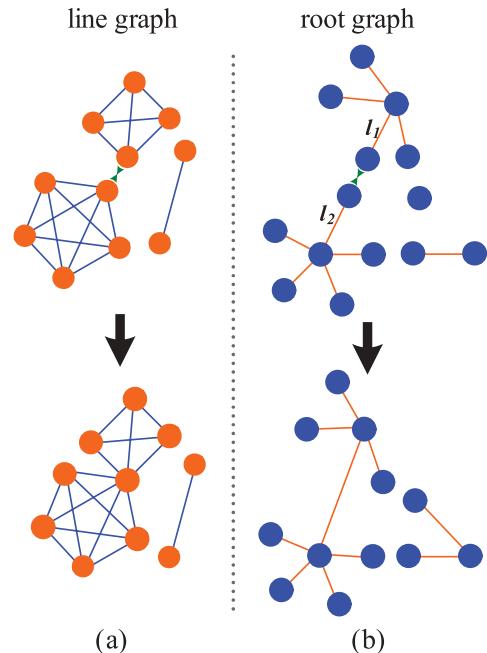


FIG. 5. (Color online) (a) The merging of two randomly selected nodes of the cliques in the line graph. (b) The corresponding root graphs before and after the nodal merging.

of t ,

$$\rho_D(G, t) = \frac{2}{CS}t - 1, \quad (7)$$

where C are the number of cliques each with S nodes.

Proof. The merging of two nodes in the line graph H , corresponds to the following operations in the root graph G (as shown in the Fig. 5): (1) choose two links l_1 and l_2 from two different complete bipartite graphs which do not share a link; (2) delete link l_1 , and delete the node with degree 1 which is incident to l_1 ; (3) delete the node with degree 1 which is incident to l_2 ; (4) let l_2 be incident to the node with degree S which was incident to l_1 . After these operations, the two nodes with degree S from two different complete bipartite graphs, are connected with a link. The degree of the remaining $C(S+1)-2$ nodes keep unchanged.

After t steps of merging in the line graph, we have that the number of nodes in the root graph $N_G = C(S+1) - 2t$, and the number of links $L_G = CS - t$. There are C nodes with degree S and $CS - 2t$ nodes with degree 1 in the root graph G . The denominator B in (3) equals

$$\begin{aligned} B &= CS^3 + (CS - 2t) - \frac{1}{2(CS-t)}(CS^2 + CS - 2t)^2 \\ &= \frac{CS(S-1)^2(CS-2t)}{2(CS-t)}. \end{aligned} \quad (8)$$

There is no degree difference among the C nodes with degree S . Each of the $(CS - 2t)$ nodes with degree 1, is adjacent with a node with degree S , therefore,

$$A = \sum_{i \sim j} (d_i - d_j)^2 = (CS - 2t)(S - 1)^2. \quad (9)$$

Substituting (8) and (9) into (3) proves Theorem 8. ■

This analytic result explains the linear increase of $\rho_D(G, t)$ with t , as shown in Fig. 4, where the root graphs of the line graphs are computed by ILIGRA, the inverse line graph construction algorithm [26], although other algorithms [27–29] can also be used. Before the first merging, $t = 0$, $\rho_D(G, t) = -1$. When $t = \frac{CS}{2}$, the root graph G is a regular graph with degree S , and $\rho_D(G, t) = 0$.

The only exception from the linear law occurs when $S = 3$, of which the assortativity coefficients of the line graphs and corresponding root graphs in the nodal merging process are shown in Fig. 4(b). The line graphs are generated by the Algorithm 1. The corresponding root graphs of the line graphs are computed by ILIGRA. The root graph of K_3 can be $K_{1,3}$ or K_3 itself. The nonlinearity in Fig. 4(b) is originated from the fact that ILIGRA picks randomly from $K_{1,3}$ and K_3 as the root graph of line graph K_3 . If we modify ILIGRA and let it always choose $K_{1,3}$ as the root graph of line graph K_3 , the linear law (7) would be fulfilled in Fig. 4(b), just like the cases when $S \neq 3$. Before the line graph becomes connected in the merging process, there are always some separate cliques K_3 in the line graph. These separate cliques K_3 are translated into $K_{1,3}$ or K_3 randomly by ILIGRA, when the corresponding root graph is computed. Hence, the root graphs do not satisfy the linear law, as shown in Fig. 4(b). However, after the line graph becomes connected in the nodal merging process, there are no separate cliques K_3 in the line graph, hence, $\rho_D(G, t)$ increases exactly linearly with $t = 58, 59, \dots, 75$, as depicted in Fig. 4(b).

The linear law offers a possibility to construct graphs with a prescribed negative assortativity ρ_D by tuning different parameters. For an arbitrary small $\varepsilon > 0$, it is always possible to construct graphs with the assortativity in the interval $(-\varepsilon + \rho_D, \varepsilon + \rho_D]$. Indeed, for an arbitrary small enough ε , it is possible to take large enough C or S (one could be fixed), such that $\varepsilon CS > 1$. For such ε, C and S , taking $t = \lfloor \frac{\varepsilon}{2}CS + (1 + \rho_D)\frac{CS}{2} \rfloor$ boils down to

$$-\frac{\varepsilon}{2}CS + (1 + \rho_D)\frac{CS}{2} < t \leq \frac{\varepsilon}{2}CS + (1 + \rho_D)\frac{CS}{2}, \quad (10)$$

as the difference of the right-hand and the left-hand sides in (10) is εCS . Relation (10) is equivalent to $-\varepsilon + \rho_D < -1 + \frac{2t}{CS} \leq \varepsilon + \rho_D$, hence we have a graph with the assortativity in the interval $(-\varepsilon + \rho_D, \varepsilon + \rho_D]$. Moreover, it is possible to find many graphs with a prescribed assortativity ρ_D : (i) by fixing the size of the clique C in one case; (ii) by fixing the number of clique S in another; or (iii) by tuning both C and S . In general, by tuning the slope $\frac{2}{CS}$, the desired negative assortativity ρ_D can be obtained.

B. Heterogeneous random line graphs with cliques of different sizes

The characteristics of assortativity of the line graphs in Sec. IV A 1 and the linear law of the assortativity presented in Theorem 8 are, however, sensitive to rather small topological changes as we exemplify in this section.

1. Random line graphs with cliques of two different sizes

We construct line graphs with cliques of two different sizes. The electrical properties of semiconductor materials can be manipulated by the addition of impurities, known as doping [30]. Inspired by doping in the semiconductor industry, we investigate the assortativity change of the line graphs after the introducing of cliques of different size. Among all the cliques we use to construct line graphs, the majority of them are of size S_m , and the rest are of size S_d , called doping cliques. As shown in Fig. 6(a), for the line graph H constructed with 40 cliques of size 4 and 10 cliques of size 6, $\rho_D(H, t)$ is very high when t is small, and $\rho_D(H, t)$ ends at value close to 0.5 when the merging process finishes. During the whole merging process, $\rho_D(H, t)$ is positive, and never close to zero. In Fig. 6(b), the line graph H is constructed with 60 cliques of size 4 and 20 cliques of size 5. The assortativity coefficient of the line graph $\rho_D(H, t)$ first decreases rapidly from almost 1 to almost 0, and after remains close to 0 for a long range of t , $\rho_D(H, t)$ starts to increase quickly and ends at value close to 0.5. The assortativity of the line graph has been raised by adding a relatively smaller number of doping cliques to the line graph.

2. Random line graphs with cliques of binomial distributed size

In this section, we construct line graphs with the cliques of binomial size S . If the size of clique S follows a binomial distribution $S \sim b(N, p)$, the probability $\Pr[S = k] = \sum_{k=0}^N \binom{N}{k} p^k (1-p)^{N-k}$. In Fig. 7(a), the line graph H is constructed with 30 cliques where $S \sim b(20, 0.3)$ and $\sum_{j=1}^C s_j = 176$. After 88 steps of merging, H becomes a line graph of 88 nodes and 490 links, with the corresponding root

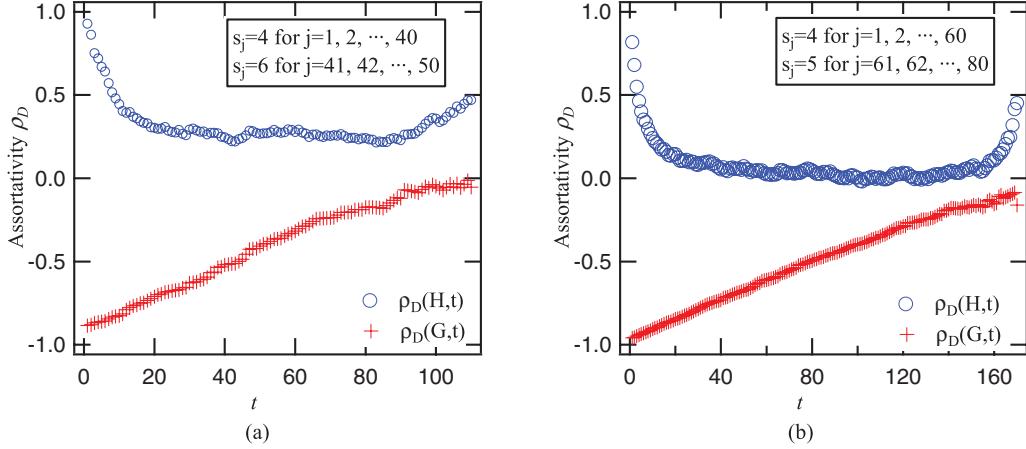


FIG. 6. (Color online) (a) The line graph H with 40 cliques of size 4 and 10 cliques of size 6, and (b) the line graph H with 60 cliques of size 4 and 20 cliques of size 5 have been constructed with Algorithm 1. The assortativity coefficient ρ_D of the line graphs and the corresponding root graphs in each merging step t is shown in this figure.

graph with 30 nodes and 88 links. In Fig. 7(b), the line graph H constructed with 50 cliques whose size follows a binomial distribution $S \sim b(20, 0.4)$ and $\sum_{j=1}^C s_j = 327$. The line graph H has 189 nodes and 1381 links, after 188 steps of merging, and the corresponding root graph G has 51 nodes and 189 links. For the 50 cliques with size $S \sim b(20, 0.4)$, the merging

process has been repeated for 1000 times, and 1000 line graphs and their root graphs were obtained. The adjacency eigenvalues of the root graphs appeared to follow a semicircle distribution, as shown in Fig. 7(c).

Both Figs. 7(a) and 7(b) illustrate that the assortativity of the line graph $\rho_D(H,t)$ at first drops from almost 1 to a certain level

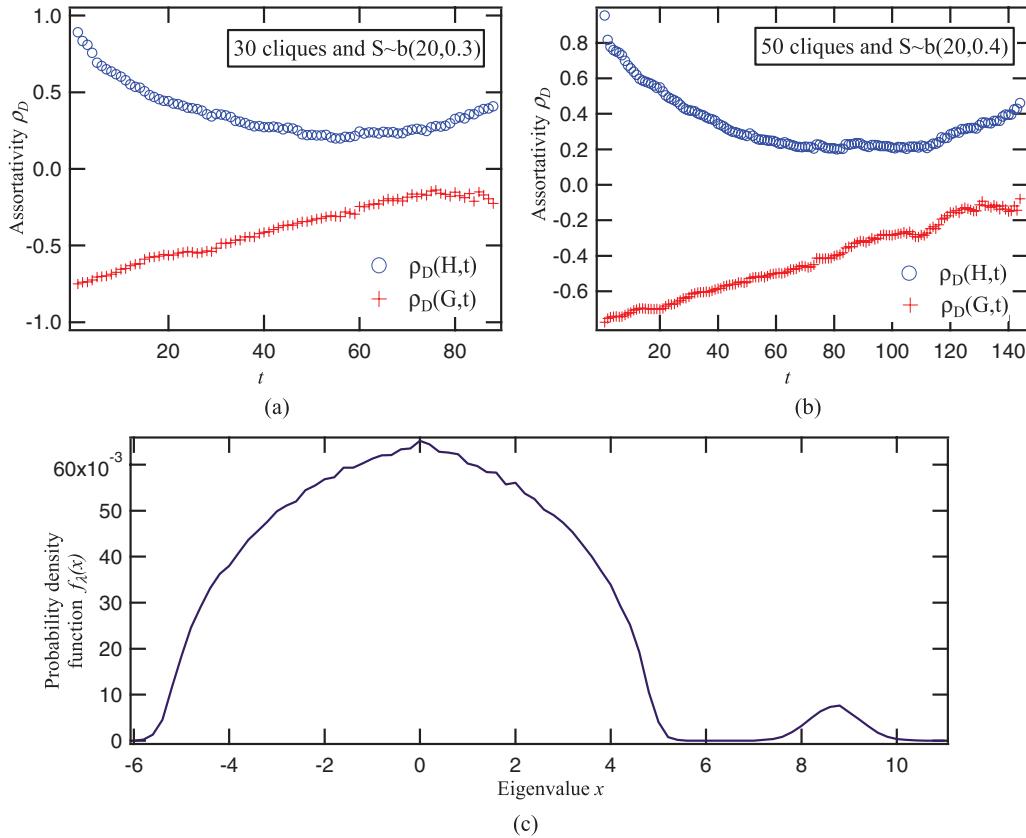


FIG. 7. (Color online) Using Algorithm 1, we construct (a) the line graph H with 30 cliques, the size of which follows a binomial distribution $S \text{ Bino}(20, 0.3)$, and (b) the line graph H with 50 cliques, the size of which follows a binomial distribution $S \text{ Bino}(20, 0.4)$. The assortativity coefficient ρ_D of the line graphs and the corresponding root graphs in each merging step t has been computed. (c) For the 50 cliques in (b), we repeat the merging process for 1000 times, and computed the probability density function of adjacency eigenvalues of the root graphs.

above 0, then it starts to increase and ends at value close to 0.5. In both numerical experiments, the assortativity coefficient of the root graph $\rho_D(G, t)$ increases steadily to a value close to 0. The adjacency eigenvalues of Erdős-Rényi random graphs follow semicircle distributions [15]. The spectrum of a graph is the unique fingerprint of that graph [31]. The root graphs of the line graphs after the merging process have binomial degree distributions, and their adjacency eigenvalues follow semicircle distributions. Hence, the root graphs are believed to be equivalent to the Erdős-Rényi random graphs.

V. CONCLUSION

Inspired by the configuration model [18,19] and Krausz's Theorem [16,17], we propose a model which can randomly generate simple graphs which are line graphs of other simple graphs. We show that consecutive integers can occur as the number of links L in the line graph $H(N, L)$. We also prove that there are multiple bands of consecutive integers, which can never appear as the number of links L in $H(N, L)$. The exact expressions of bands and bandgaps of L have been derived.

Our model constructs line graphs by merging step by step a pair of nodes of the cliques, which we use to construct line graphs. Obeying necessary rules to ensure that the resulting graphs are line graphs, two nodes to be merged are randomly chosen at each step. If the cliques are all of the same size, the assortativity of the line graphs of each step are close to 0, and the assortativity of the corresponding root graphs increases linearly from -1 to 0 with the steps of merging nodes. With the linear function ρ_D of the step t in Theorem 8, a graph with a prescribed negative assortativity coefficient can be constructed. The largest eigenvalue $\lambda_1(A)$ of the adjacency matrix A of a network is the only factor of the lower bound $\tau_c^{(1)}$ of the network's epidemic threshold τ_c , $\tau_c^{(1)} = \frac{1}{\lambda_1(A)} \leq \tau_c$. The largest eigenvalue $\lambda_1(A)$ can be adjusted by tuning the assortativity coefficient ρ_D . The linear law for the assortativity provides a new method to tune the assortativity besides the method of degree-preserving rewiring. If we "dope" the constructing elements of the line graphs—the cliques of the same size—with a relatively smaller number of cliques of different size, the characteristics of the assortativity of the line graphs is completely altered. We also generate line graphs with the cliques whose sizes follow a binomial distribution. The corresponding root graphs, with binomial degree distributions, zero assortativity and semicircle eigenvalue distributions, are equivalent to Erdős-Rényi random graphs.

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APPENDIX A: PROOF OF THEOREM 4

The only element $\binom{N}{2}$ in V_1 is the number of links in the line graph $H(N, L)$ when the line graph H is a complete graph K_N . Next, we prove that L is the number of links in $H(N, L)$ if L is an integer and $L \in \bigcup_{k=2}^{\lfloor \frac{N+1}{2} \rfloor} V_k$. When $H(N, L)$ contains

the principal clique K_{N-k+1} and the clique K_k , sharing node k , as shown in Fig. 2(a), the number of links L can take the consecutive numbers in $\{(\binom{N-k+1}{2}) + \binom{k}{2}, \dots, (\binom{N-k+1}{2}) + \binom{k}{2} + (k-1)\}$, since each of the other $k-1$ nodes in K_k can be connected by a link to a node in K_{N-k+1} . Similarly, when $H(N, L)$ is constructed by two cliques K_{N-k+1} and K_{k-1} and an isolated node, the number of links L can take the consecutive numbers in $\{(\binom{N-k+1}{2}) + \binom{k-1}{2}, \dots, (\binom{N-k+1}{2}) + \binom{k-1}{2} + (k-2)\}$, as shown in Fig. 2(b). In general, if $H(N, L)$ is constructed by two cliques K_{N-k+1} and K_j ($2 \leq j \leq k$), which have node k in common, and $k-j$ isolated nodes, all the integers in the set $W_j = \{(\binom{N-k+1}{2}) + \binom{j}{2}, \dots, (\binom{N-k+1}{2}) + \binom{j}{2} + (j-1)\}$ can occur as the number of links L in the line graph $H(N, L)$. The case $j=2$ is shown in Fig. 2(c), while in Fig. 2(d), there is only a clique of K_{N-k+1} and $k-1$ isolated nodes in $H(N, L)$, the number of links can be only $L = \binom{N-k+1}{2}$. We define

$W_1 = \{(\binom{N-k+1}{2})\}$. For $3 \leq j \leq k$, the smallest element of W_j , $(\binom{N-k+1}{2}) + \binom{j}{2}$, equals the largest element of W_{j-1} plus 1, $(\binom{N-k+1}{2}) + \binom{j-1}{2} + (j-2) + 1$,

$$\begin{aligned} & \binom{N-k+1}{2} + \binom{j-1}{2} + (j-2) + 1 \\ &= \binom{N-k+1}{2} + \binom{j}{2}. \end{aligned}$$

The smallest element of W_2 equals the element of W_1 plus 1, $(\binom{N-k+1}{2}) + 1$,

$$\binom{N-k+1}{2} + 1 = \binom{N-k+1}{2} + \binom{2}{2}.$$

Hence,

$$\begin{aligned} V_k &= \left\{ \binom{N-k+1}{2}, \dots, \binom{N-k+1}{2} + \binom{k}{2} + (k-1) \right\} \\ &= \bigcup_{j=1}^k W_j, \end{aligned}$$

where $2 \leq k \leq \lfloor \frac{N+1}{2} \rfloor$. Thus, all the integers in the sets $\bigcup_{k=2}^{\lfloor \frac{N+1}{2} \rfloor} V_k$ can occur as the number of links L .

Lemma 3 states that, for each k between 2 and $\lfloor \frac{N+1}{2} \rfloor$ (the size of the principal clique is $N-k+1$), the set V_k covers the minimum and maximum number of links in $H(N, L)$. Hence, all the integers in the intervals $\Psi_k = \{(\binom{N-k}{2}) + \binom{k+1}{2} + k + 1, \dots, (\binom{N-k+1}{2}) - 1\}$, which are the gaps between V_{k+1} and V_k , $1 \leq k \leq \lfloor \frac{N+1}{2} \rfloor - 1$, cannot occur as the number of links L in $H(N, L)$.

In the following, we prove that all the integers in the set $\{0, 1, \dots, (\lfloor \frac{N+1}{2} \rfloor) + \lfloor \frac{N+1}{2} \rfloor - 1\}$ can occur as the number of links L . Taking $k = \lfloor \frac{N+1}{2} \rfloor$, we employ the same method which is used to prove the integers in V_k can occur as L , except deleting all the links in the principal clique K_{N-k+1} . For $2 \leq j \leq \lfloor \frac{N+1}{2} \rfloor$, suppose that $H(N, L)$ is constructed by a clique K_j consisting of nodes $n_k, n_{k-1}, \dots, n_{k-j+1}$, isolated nodes n_1, n_2, \dots, n_{k-j} , and the set of nodes $n_{k+1}, n_{k+2}, \dots, n_N$,

among which any pair of nodes are not adjacent. The number of links L can take any integer in $\{\binom{j}{2}, \dots, \binom{j}{2} + (j-1)\}$, since each of nodes $n_k, n_{k-1}, \dots, n_{k-j+1}$ can be connected by a link to a node in $\{n_{k+1}, n_{k+2}, \dots, n_N\}$, where $\binom{a}{b} = 0$ if $a, b \in \mathbb{N}$ and $a < b$. We further have $\{0, 1, 2, 3, \dots, (\lfloor \frac{N+1}{2} \rfloor) + \lfloor \frac{N+1}{2} \rfloor - 1\} = \bigcup_{j=1}^{\lfloor \frac{N+1}{2} \rfloor} \{\binom{j}{2}, \dots, \binom{j}{2} + (j-1)\}$. Hence, all the integers in the set $\{0, 1, 2, \dots, (\lfloor \frac{N+1}{2} \rfloor) + \lfloor \frac{N+1}{2} \rfloor - 1\}$ can occur as the number of links L .

If N is odd, $(\lfloor \frac{N+1}{2} \rfloor) + \lfloor \frac{N+1}{2} \rfloor - 1 = (\frac{N+1}{2}) + \frac{N+1}{2} - 1$ and the smallest element of $V_{\lfloor \frac{N+1}{2} \rfloor}$, $(N - \lfloor \frac{N+1}{2} \rfloor + 1) = (\frac{N+1}{2}) + \frac{N+1}{2}$. If N is even, $(\lfloor \frac{N+1}{2} \rfloor) + \lfloor \frac{N+1}{2} \rfloor - 1 = (\frac{N+1}{2}) + \frac{N+1}{2}$

$\frac{N}{2} - 1$, and the smallest element of $V_{\lfloor \frac{N+1}{2} \rfloor}$, $(N - \lfloor \frac{N+1}{2} \rfloor + 1) = (\frac{N}{2} + 1) = (\frac{N}{2}) + \frac{N}{2}$. Hence, there is no gap between the set $\{0, 1, 2, \dots, (\lfloor \frac{N+1}{2} \rfloor) + \lfloor \frac{N+1}{2} \rfloor - 1\}$ and $V_{\lfloor \frac{N+1}{2} \rfloor}$.

We have proven that (i) all the integers in $\bigcup_{k=1}^{\lfloor \frac{N+1}{2} \rfloor} V_k$ can occur as L , and (ii) all the integers in $\{0, 1, 2, \dots, (\lfloor \frac{N+1}{2} \rfloor) + \lfloor \frac{N+1}{2} \rfloor - 1\}$ can occur as L , and (iii) all the natural numbers in the gaps between $V_{\lfloor \frac{N+1}{2} \rfloor}, V_{\lfloor \frac{N+1}{2} \rfloor + 1}, \dots, V_1$, cannot occur as L , and (iv) there is no gap between $\{0, 1, 2, \dots, (\lfloor \frac{N+1}{2} \rfloor) + \lfloor \frac{N+1}{2} \rfloor - 1\}$ and $V_{\lfloor \frac{N+1}{2} \rfloor}$. All these conclusions together prove Theorem 4.

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