Deterministic Hierarchical Networks *

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Abstract

It has been shown that many networks associated with complex systems are small-world (they have both a large local clustering coefficient and a small diameter) and they are also scale-free (the degrees are distributed according to a power law). Moreover, these networks are very often hierarchical, as they describe the modularity of the systems that are modeled. Most of the studies for complex networks are based on stochastic methods. However, a deterministic method, with an exact determination of the main relevant parameters of the networks, has proven useful. Indeed, this approach complements and enhances the probabilistic and simulation techniques and, therefore, it provides a better understanding of the modeled systems. In this paper we find the radius, diameter, clustering coefficient and degree distribution of a generic family of deterministic hierarchical small-world scale-free networks that has been considered for modeling real-life complex systems.

Keywords: Hierarchical network; Small-word; Scale-free; Degree; Diameter; Clustering.

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1 Introduction

With the publication in 1998 and 1999 of the papers by Watts and Strogatz on small-world networks [31] and by Barabási and Albert on scale-free networks [5], there has been a renewed interest in the study of networks associated to complex systems that has received a considerable boost as an interdisciplinary subject, see [30] .

Many real-life networks, transportation and communication systems (including the power distribution and telephone networks), Internet [15], World Wide Web [4], and several social and biological networks [17, 18, 21], belong to a class of networks known as small-world scale-free networks. All these networks exhibit both a strong local clustering coefficient (nodes have many mutual neighbors) and a small diameter. Another important characteristic is that the number of links attached to the nodes usually obeys a power law distribution ('scale-free' network). Several authors also noticed that the modular structure of a network can be characterized by a specific clustering distribution that depends on the degree. The network is then called hierarchical [26, 28, 32]. Moreover, with the introduction of a new measuring technique for graphs, it has been discovered that many real networks can also be categorized as self-similar, see [27].

Along with these observational studies, researchers have developed different models [3, 14, 22], most of them stochastic, which should help to understand and predict the behavior and characteristics of complex systems. However, new deterministic models constructed by recursive methods, based on the existence of 'cliques' (clusters of nodes linked to each other), have also been introduced [7, 10, 13, 19, 33]. Such deterministic models have the advantage that they allow one to analytically compute relevant properties and parameters, which may be compared with data from real and simulated networks. In [7], Barabási *et al.* proposed a simple hierarchical family of deterministic networks and showed it had a small-world scale-free nature. However, their null clustering coefficient of all the vertices (the clustering coefficient of a vertex is defined as the number of edges between the neighbors of this vertex divided by the number of all possible edges between these neighbors) contrasts with many real networks that have a high clustering coefficient. Another family of hierarchical networks is proposed in [26]. It combines a modular structure with a scale-free topology and models the metabolic networks of living organisms and networks associated with generic system-level cellular organizations. A simple variation of this hierarchical network is considered in [25], where other modular networks (as WWW, the actor network, Internet at the domain level, etc.) are studied. This model is further generalized in [24].

Several authors [6, 25, 26] claim that a signature for a hierarchical network on top of the small-world scale-free characteristics is that the clustering of the vertices of the graph follows $C(k_i) \propto 1/k_i$, where k_i is the degree of vertex i.

Other more recent examples of recursively grown, deterministic hierarchical networks, and examples of how these topological features may affect processes embedded on them are the following: First, there is a very interesting class of deterministic hierarchical networks, originally introduced by Dyson [12], that has recently been investigated by Agliari et al. [1, 2]. Moreover, the original graph introduced by Ravasz et al. [25, 26] (as well as the one by Song, Havlin, and Makse [27]) has been extensively investigated in the context of reaction-diffusion processes, see for instance Meyer et al. [20] and Tavani and Agliari [29].

In this paper, we present a new family of deterministic hierarchical networks, which generalizes some previous proposals [26, 25, 24, 9, 8].

The generalization is carried out in three fronts: First, it concerns with the building procedure, as the obtained graphs are defined as graphs on alphabets [16], where vertices are labeled with words on a given alphabet, and the edges are defined by a specific rule relating different words. Second, some new edges are added between some specific vertices (called roots), which enables to reduce the diameter and the mean distance of the resulting structure. Third, our approach allows to use basic building blocks (complete graphs) with different numbers of vertices, so obtaining similar results. In fact, this has been studied in a subsequent work by the last two authors [11], where a simple routing algorithm is presented.

Here, and as a first approach, our family of hierarchical networks is defined recursively from an initial complete graph on n vertices. Then, a more formal definition is introduced by using the above mentioned technique of graphs on alphabets. This allows us the characterization of their main distance-related parameters, such as the radius and the diameter, and the degree and clustering distributions are also determined. Moreover, we have seen that they are scale-free with a power law exponent, which depends on the initial complete graph; that the clustering distribution $c(z)$ scales with the degree as z^{-1}; and that the clustering coefficient does not depend on the order of the graph, as in many networks associated to real systems [6, 25, 26].

2 The hierarchical graph $H_{n,k}$

In this section we generalize the constructions of deterministic hierarchical graphs introduced by Ravasz *et al.* [25, 26] and Noh [24]. Roughly speaking, these graphs are constructed first by connecting a selected root vertex of a complete graph K_n to some vertices of $n-1$ replicas of K_n, and establishing also some edges between such copies of K_n. This gives a graph with n^2 vertices. Next, $n-1$ replicas of the new whole structure are added, again with some edges between them and to the same root vertex. At this step the graph has n^3 vertices. Then we iterate the process until, for some integer $k \geq 1$, the desired graph order n^k is reached (see below for a formal definition). Our model enhances the modularity and self-similarity of the graph obtained, and allows us to derive exact expressions for the radius, diameter, degree and clustering distributions.

2.1 Definition, order and size

Next we provide a recursive formal definition of the proposed family of graphs, characterized by the parameters n (order of the initial complete graph) and k (number of iterations or dimension). This allows us to give also a direct definition and derive an expression for the number of edges (the radius and the diameter will be studied in the next section).

Definition 2.1 *Let n and k be positive integers, $n \geq 2$ and $k \geq 1$. The hierarchical graph $H_{n,k}$ has vertex set $V_{n,k}$, with n^k vertices, denoted by the k-tuples $x_1x_2x_3\dots x_k$, $x_i \in \mathbb{Z}_n$, for $1 \leq i \leq k$, and edge set $E_{n,k}$ defined recursively as follows:*

- *$H_{n,1}$ is the complete graph K_n.*
- *For $k > 1$, $H_{n,k}$ is obtained from the union of n copies of $H_{n,k-1}$, each denoted by $H^{\alpha}_{n,k-1}$, for $0 \leq \alpha \leq n-1$, and with vertices $x^{\alpha}_2 x^{\alpha}_3 \dots x^{\alpha}_k \equiv \alpha x_2 x_3 \dots x_k$, by adding the following new edges (where adjacencies are denoted by '$\sim$'):*

$$000\dots00 \sim x_1x_2x_3\dots x_{k-1}x_k, \qquad x_j \neq 0,\ 1 \leq j \leq k; \tag{1}$$

$$x_100\dots00 \sim y_100\dots00, \qquad x_1, y_1 \neq 0,\ x_1 \neq y_1. \tag{2}$$

Alternatively, a direct definition of the edge set $E_{n,k}$ is given by the following adjacency rules (when $i = 0$, then $x_1x_2\dots x_i$ is the empty string):

$$x_1x_2\dots x_k \sim x_1x_2\dots x_{k-1}y_k, \quad y_k \neq x_k; \tag{3}$$

$$x_1x_2\dots x_i00\dots0 \sim x_1x_2\dots x_ix_{i+1}x_{i+2}\dots x_k, \quad x_j \neq 0,\ i+1 \leq j \leq k,\ 0 \leq i \leq k-2; \tag{4}$$

$$x_1x_2\dots x_i00\dots0 \sim x_1x_2\dots x_{i-1}y_i00\dots0, \quad x_i, y_i \neq 0,\ y_i \neq x_i,\ 1 \leq i \leq k-1. \tag{5}$$

Notice that both conditions (1) and (2) of the recursive definition correspond to (4) with $i = 0$, and (5) with $i = 1$, respectively.

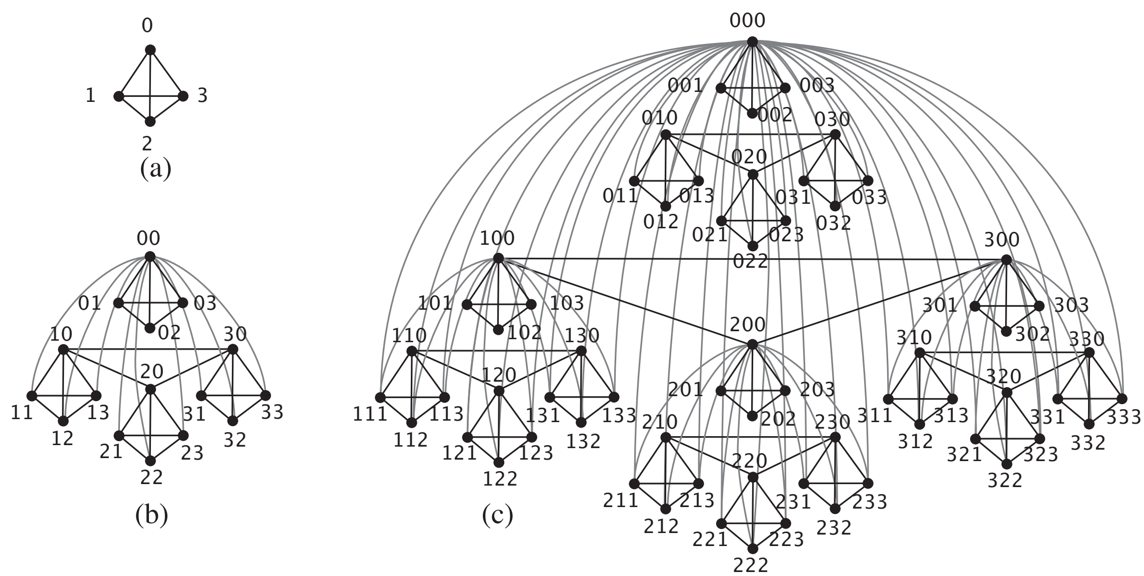

Figure 1: Hierarchical graphs with initial order 4: (a) $H_{4,1}$, (b) $H_{4,2}$, (c) $H_{4,3}$.

To illustrate our construction, Fig. 1 shows the hierarchical graphs $H_{4,k}$, for $k = 1, 2, 3$. The following result gives the number of edges of $H_{n,k}$, which can be easily computed by using the recursive definition.

Proposition 2.2 *The size of* $H_{n,k}$ *is*

$$|E_{n,k}| = \frac{3}{2}n^{k+1} - (n-1)^{k+1} - 2n^k - \frac{n}{2} + 1. \tag{6}$$

Proof. When constructing $H_{n,k}$ from n copies of $H_{n-1,k}$, the adjacencies (1) and (2) introduce $(n-1)^k$ and $\binom{n-1}{2}$ new edges, respectively. Therefore,

$$|E_{n,k}| = n|E_{n,k-1}| + (n-1)^k + \binom{n-1}{2}.$$

By applying recursively this formula and taking into account that $|E_{n,1}| = \binom{n}{2}$, we get

$$|E_{n,k}| = n^{k-1}\binom{n}{2} + \sum_{i=2}^{k} n^{k-i}(n-1)^i + \binom{n-1}{2}\sum_{i=0}^{k-2} n^i, \tag{7}$$

which yields the result. $\square$

2.2 Hierarchical properties

The hierarchical properties of the graphs $H_{n,k}$ are summarized by the following facts, that are a direct consequences of the definition:

(a) According to (3), for each sequence of fixed values $\alpha_i \in \mathbb{Z}_n$, $1 \le i \le k-1$, the vertex set $\{\alpha_1\alpha_2 \dots \alpha_{k-1}x_k : x_k \in \mathbb{Z}_n\}$ induces a subgraph isomorphic to K_n.

(b) Vertex $\boldsymbol{r} := 00\dots0$, which we distinguish and call *root*, is adjacent by (4) to vertices $x_1x_2\dots x_k$, $x_i \neq 0$, for all $1 \le i \le k$, which we call *peripheral*.

(c) For every i, $1 \le i \le k-1$, $H_{n,k}$ can be decomposed into n^i vertex-disjoint subgraphs isomorphic to $H_{n,k-i}$. Each of such (induced) subgraphs is denoted by $H^{\boldsymbol{\alpha}}_{n,k-i}$ and has vertex labels $\boldsymbol{\alpha}x_{i+1}x_{i+2}\dots x_k$, with $\boldsymbol{\alpha} = \alpha_1\alpha_2\dots\alpha_i \in \mathbb{Z}_n^i$ being a fixed sequence. In particular, for $i=1$, $H_{n,k}$ has n subgraphs $H^{\alpha}_{n,k-1}$, $\alpha = 0, 1, \dots, n-1$, as stated in the recursive definition.

(d) The root vertex of the subgraph $H^{\boldsymbol{\alpha}}_{n,k-i}$ is $\boldsymbol{\alpha}\underbrace{00\dots0}_{k-i}$. Thus, the total number of root vertices of all the subgraphs, including the one in $H_{n,k}$, is

$$1 + (n-1)\sum_{i=1}^{k-1} n^{i-1} = n^{k-1}, \tag{8}$$

as expected since a given vertex $x_1x_2\dots x_k$ is a root (of some subgraph) if and only if $x_k = 0$.

(e) The peripheral vertices of the subgraph $H^{\boldsymbol{\alpha}}_{n,k-i}$ are of the form $\boldsymbol{\alpha}x_{i+1}x_{i+2}\dots x_k$, where $x_j \neq 0$ and $i+1 \le j \le k$. Thus, the total number of peripheral vertices of all the subgraphs, including those in $H_{n,k}$, see (b), is

$$(n-1)^k + (n-1)\sum_{i=1}^{k-1} n^{i-1}(n-1)^{k-i} = n^{k-1}(n-1), \tag{9}$$

as expected, since $x_1x_2\dots x_k$ is a peripheral vertex (of some subgraph) if and only if $x_k \neq 0$. Note that, adding up (8) and (9), we get $n^k = |V_{n,k}|$, so that every vertex of $H_{n,k}$ is a root or peripheral of some subgraph isomorphic to $H_{n,k'}$, for $1 \le k' \le k$.

(f) By collapsing in $H_{n,k}$ each of the n^i subgraphs $H^{\boldsymbol{\alpha}}_{n,k-i}$, $\boldsymbol{\alpha} \in \mathbb{Z}_n^i$, into a single vertex and all multiple edges into one, we obtain a graph isomorphic to $H_{n,i}$.

(g) According to (5), for every fixed i, $1 \le i \le k$, and given a sequence $\boldsymbol{\alpha} \in \mathbb{Z}_n^{i-1}$, there exist all possible edges among the $n-1$ vertices labeled $\boldsymbol{\alpha} x_i 00\ldots 0$ with $x_i \in \mathbb{Z}_n^* = \{1, 2, \ldots, n-1\}$, that is, the root vertices of $H_{n,k-i}^{\boldsymbol{\alpha} x_i}$. Thus, these edges induce a complete graph isomorphic to K_{n-1}.

3 Radius and Diameter

In this section we determine the radius and diameter of $H_{n,k}$ by using a recursive method. With this aim, let us first introduce some notation concerning $H_{n,k}$. Let $\partial_k(\boldsymbol{x}, \boldsymbol{y})$ denote the distance between vertices $\boldsymbol{x}, \boldsymbol{y} \in V_{n,k}$ in $H_{n,k}$; and $\partial_k(\boldsymbol{x}, U) := \min_{\boldsymbol{u} \in U}\{\partial_k(\boldsymbol{x}, \boldsymbol{u})\}$. Let $\boldsymbol{r}^\alpha = \alpha 00\ldots 0$ be the root vertex of $H_{n,k-1}^\alpha$, for $\alpha \in \mathbb{Z}_n$ (as stated before, $\boldsymbol{r}$ stands for the root vertex of $H_{n,k}$). Let P and P^α, for $\alpha \in \mathbb{Z}_n$, denote the set of peripheral vertices of $H_{n,k}$ and $H_{n,k-1}^\alpha$, respectively.

Proposition 3.1 *Let r_k, $\varepsilon_k(\boldsymbol{r})$, and D_k denote, respectively, the radius, the eccentricity of the root $\boldsymbol{r}$, and the diameter of $H_{n,k}$. Then,*

(a) $r_k = \varepsilon_k(\boldsymbol{r}) = k$.

(b) $D_k = 2k - 1$.

Proof.

(a) The radius of $H_{n,k}$ coincides with the eccentricity of the root: $r_k = \varepsilon_k(\boldsymbol{r}) = k$.

(b) By induction on k.
For $k = 1$: As $H_{n,1} = K_n$, then $D_1 = 1$.
Assume that, for some fixed $k > 1$, $D_k = 2k - 1$.
Then, for $k' = k + 1$: As $H_{n,k'}$ is made from n copies of $H_{n,k}$ (called copy 0, copy 1,…, copy $n-1$), two further vertices in $H_{n,k'}$ must be in different copies of $H_{n,k}$. If none of these two vertices is in the copy 0 of $H_{n,k}$, then both copies are joined by their roots. Then, the diameter of $H_{n,k'}$ is:

$$D_{k'} = \varepsilon_k(\boldsymbol{r}) + \varepsilon_k(\boldsymbol{r}) + 1 = 2k + 1 = 2k' - 1,$$

where $\boldsymbol{r}$ is the root of any of the two copies of $H_{n,k}$. On the other hand, if one of the two vertices is in the copy 0 of $H_{n,k}$, then both copies are joined from the root of the copy 0 to the peripheral vertices of the other copy of $H_{n,k}$. Then, the diameter of $H_{n,k'}$ is:

$$D_{k'} = \varepsilon_k(\boldsymbol{r}) + \varepsilon_k(\boldsymbol{p}) + 1 = 2k + 1 = 2k' - 1,$$

where $\boldsymbol{p}$ is one of the peripheral vertices of the non-zero copy of $H_{n,k}$, and $\varepsilon_k(\boldsymbol{p}) = k$.

□

Then, from the result on the diameter and property (c) in Subsection 2.2, we have that the distance between two vertices $\boldsymbol{x}$ and $\boldsymbol{y}$ of $H_{n,k}$, with maximum common prefix of length $i = |\boldsymbol{x} \cap \boldsymbol{y}|$, satisfies

$$\partial(\boldsymbol{x}, \boldsymbol{y}) \leq 2(k-i) - 1.$$

Alternatively, we can give recursive proofs of these results. Indeed, let us consider the case of the diameter. With this aim, we first give the following result that follows from the recursive definition of $H_{n,k}$:

Lemma 3.2 *Let $\boldsymbol{x}$ and $\boldsymbol{y}$ be two vertices in $H_{n,k}$, for $k > 1$. Then, depending on the subgraphs $H_{n,k-1}$ where such vertices belong to, we are in one of the following three cases:*

(a) *If $\boldsymbol{x}, \boldsymbol{y} \in V^{\alpha}_{n,k-1}$ for some $\alpha \in \mathbb{Z}_n$, that is, $\boldsymbol{x} = \alpha\boldsymbol{x}'$ and $\boldsymbol{y} = \alpha\boldsymbol{y}'$, then*

$$\partial_k(\boldsymbol{x}, \boldsymbol{y}) = \partial_{k-1}(\boldsymbol{x}', \boldsymbol{y}').$$

(b) *If $\boldsymbol{x} \in V^{0}_{n,k-1}$ and $\boldsymbol{y} \in V^{\alpha}_{n,k-1}$ for some $\alpha \in \mathbb{Z}^*_n$, that is $\boldsymbol{x} = 0\boldsymbol{x}'$, $\boldsymbol{y} = \alpha\boldsymbol{y}'$, with $\alpha \neq 0$, then*

$$\partial_k(\boldsymbol{x}, \boldsymbol{y}) = \partial_{k-1}(\boldsymbol{x}', \boldsymbol{r}^0) + 1 + \partial_{k-1}(\boldsymbol{y}', P^{\alpha}).$$

(c) *If $\boldsymbol{x} \in V^{\alpha}_{n,k-1}$ and $\boldsymbol{y} \in V^{\beta}_{n,k-1}$ for some $\alpha, \beta \in \mathbb{Z}^*_n$, $\alpha \neq \beta$, that is $\boldsymbol{x} = \alpha\boldsymbol{x}'$, $\boldsymbol{y} = \beta\boldsymbol{y}'$, with $\alpha, \beta \neq 0$, then*

$$\partial_k(\boldsymbol{x}, \boldsymbol{y}) = \min\{\partial_{k-1}(\boldsymbol{x}', P^{\alpha}) + 2 + \partial_{k-1}(\boldsymbol{y}', P^{\beta}),\ \partial_{k-1}(\boldsymbol{x}', \boldsymbol{r}^{\alpha}) + 1 + \partial_{k-1}(\boldsymbol{r}^{\beta}, \boldsymbol{y}')\}.$$

Lemma 3.3 *For any vertex $\boldsymbol{x}$ in $H_{n,k}$ we have:*

$$\partial_k(\boldsymbol{x}, \boldsymbol{r}) \leq \begin{cases} k-1 & \text{if } \boldsymbol{x} = 0\boldsymbol{x}', \\ k & \text{otherwise,} \end{cases} \qquad \text{and} \qquad \partial_k(\boldsymbol{x}, P) \leq \begin{cases} k & \text{if } \boldsymbol{x} = 0\boldsymbol{x}', \\ k-1 & \text{otherwise.} \end{cases}$$

Proof. By induction on k.
Case $k = 1$: If $\boldsymbol{x} = \boldsymbol{0} = \boldsymbol{r}$, then $\partial_1(\boldsymbol{x}, \boldsymbol{r}^0) = 0$ and $\partial_1(\boldsymbol{x}, P) = 1$. Otherwise,

$\boldsymbol{x} \in P = \mathbb{Z}_n^*$, and then $\partial_1(\boldsymbol{x}, \boldsymbol{r}) = 1$ and $\partial_1(\boldsymbol{x}, P) = 0$.
Case $k > 1$: We observe that, from the recursive definition of $H_{n,k}$,

$$\partial_k(\boldsymbol{x}, \boldsymbol{r}) = \begin{cases} \partial_{k-1}(\boldsymbol{x}', \boldsymbol{r}^0) & \text{if } \boldsymbol{x} = 0\boldsymbol{x}', \\ \partial_{k-1}(\boldsymbol{x}', P^\alpha) + 1 & \text{if } \boldsymbol{x} = \alpha\boldsymbol{x}' \text{ and } \alpha \neq 0, \end{cases}$$

and

$$\partial_k(\boldsymbol{x}, P) = \begin{cases} \partial_{k-1}(\boldsymbol{x}', \boldsymbol{r}^0) + 1 & \text{if } \boldsymbol{x} = 0\boldsymbol{x}', \\ \partial_{k-1}(\boldsymbol{x}', P^\alpha) & \text{if } \boldsymbol{x} = \alpha\boldsymbol{x}' \text{ and } \alpha \neq 0. \end{cases}$$

Then, by the induction hypothesis, the lemma holds. □

In the next result, $\boldsymbol{z}^{01} = 0101\ldots$ and $\boldsymbol{z}^{10} = 1010\ldots$ denote any vertex $x_1x_2\ldots x_i\ldots$ of $H_{n,k}$ or $H_{n,k-1}$, where $x_i \equiv i+1 \pmod 2$ and $x_i \equiv i \pmod 2$, respectively.

Lemma 3.4 *In $H_{n,k}$, the following equalities hold:*

(a) $\partial_k(\boldsymbol{z}^{01}, \boldsymbol{r}) = \partial_k(\boldsymbol{z}^{10}, P) = k - 1,$

(b) $\partial_k(\boldsymbol{z}^{10}, \boldsymbol{r}) = \partial_k(\boldsymbol{z}^{01}, P) = k.$

Proof. By induction on k.
Case $k = 1$: $H_{n,k}$ is the complete graph K_n, and the result clearly holds.
Case $k > 1$: From Lemma 3.2 we have:

(a) $\partial_k(\boldsymbol{z}^{01}, \boldsymbol{r}) = \partial_{k-1}(\boldsymbol{z}^{10}, \boldsymbol{r}^0) = k - 1,$

$\partial_k(\boldsymbol{z}^{10}, P) = \partial_{k-1}(\boldsymbol{z}^{01}, P^0) = k - 1;$

(b) $\partial_k(\boldsymbol{z}^{10}, \boldsymbol{r}) = \partial_{k-1}(\boldsymbol{z}^{01}, P^1) + 1 = k,$

$\partial_k(\boldsymbol{z}^{01}, P) = \partial_{k-1}(\boldsymbol{z}^{10}, \boldsymbol{r}^0) + 1 = k - 1 + 1 = k.$

□

Now we can give the result about the diameter of $H_{n,k}$.

Proposition 3.5 *The diameter of $H_{n,k}$ is $D_k = 2k - 1$.*

Proof. First we prove by induction on k that, for any given pair of vertices of $H_{n,k}$, $\boldsymbol{x}$ and $\boldsymbol{y}$, we have $\partial_k(\boldsymbol{x}, \boldsymbol{y}) \leq 2k - 1$.
Case $k = 1$: The result trivially holds since $H_{n,1} = K_n$ and $D_1 = 1$.
Case $k > 1$: Considering the three cases of Lemma 3.2 and by using the induction hypothesis, we have:

(*a*) If $\boldsymbol{x}, \boldsymbol{y} \in V^{\alpha}_{n,k-1}$ for some $\alpha \in \mathbb{Z}_n$, that is, $\boldsymbol{x} = \alpha\boldsymbol{x'}$ and $\boldsymbol{y} = \alpha\boldsymbol{y'}$, then,

$$\partial_k(\boldsymbol{x}, \boldsymbol{y}) = \partial_{k-1}(\boldsymbol{x'}, \boldsymbol{y'}) \leq 2(k-1) - 1 = 2k - 3 < 2k - 1.$$

(*b*) If $\boldsymbol{x} \in V^{0}_{n,k-1}$ and $\boldsymbol{y} \in V^{\alpha}_{n,k-1}$ for some $\alpha \in \mathbb{Z}^*_n$, that is, $\boldsymbol{x} = 0\boldsymbol{x'}$, $\boldsymbol{y} = \alpha\boldsymbol{y'}$, with $\alpha \neq 0$, then,

$$\partial_k(\boldsymbol{x}, \boldsymbol{y}) = \partial_{k-1}(\boldsymbol{x'}, \boldsymbol{r}^0) + 1 + \partial_{k-1}(\boldsymbol{y'}, P^{\alpha}) \leq 2(k-1) + 1 = 2k - 1,$$

since, by Lemma 3.3, $\partial_{k-1}(\boldsymbol{x'}, \boldsymbol{r}^0) \leq k - 1$ and $\partial_{k-1}(\boldsymbol{y'}, P^{\alpha}) \leq k - 1$.

(*c*) If $\boldsymbol{x} \in V^{\alpha}_{n,k-1}$ and $\boldsymbol{y} \in V^{\beta}_{n,k-1}$ for some $\alpha, \beta \in \mathbb{Z}^*_n$, $\alpha \neq \beta$, that is $\boldsymbol{x} = \alpha\boldsymbol{x'}$, $\boldsymbol{y} = \beta\boldsymbol{y'}$, with $\alpha, \beta \neq 0$, then

$$\begin{aligned}\partial_k(\boldsymbol{x}, \boldsymbol{y}) &= \min\{\partial_{k-1}(\boldsymbol{x'}, P^{\alpha}) + 2 + \partial_{k-1}(\boldsymbol{y'}, P^{\beta}),\ \partial_{k-1}(\boldsymbol{x'}, \boldsymbol{r}^{\alpha}) + 1 + \partial_{k-1}(\boldsymbol{r}^{\beta}, \boldsymbol{y'})\} \\ &\leq 2(k-1) + 1 = 2k - 1,\end{aligned}$$

since, by Lemma 3.4, $\partial_{k-1}(\boldsymbol{x'}, \boldsymbol{r}^{\alpha}) \leq k - 1$ and $\partial_{k-1}(\boldsymbol{r}^{\beta}, \boldsymbol{y'}) \leq k - 1$.

Now, we have to prove that there exist two vertices in $H_{n,k}$ at distance exactly $2k - 1$. Let $\boldsymbol{x} = \boldsymbol{z}^{01}$ and $\boldsymbol{y} = \boldsymbol{z}^{10}$. It follows from Lemmas 3.2 and 3.4 that $\partial_k(\boldsymbol{x}, \boldsymbol{y}) = 2k - 1$. This completes the proof. □

Note that the diameter scales logarithmically with the order $N = |V_{n,k}| = n^k$, since $D_k = \frac{2}{\log n} \log N - 1$. This property, together with the high value of the clustering coefficient (see next section), shows that this is a small-world network.

4 Degree and clustering distribution

In this section we study the degree and clustering distributions of the graph $H_{n,k}$.

Proposition 4.1 *The vertex degree distribution in $H_{n,k}$ is as follows:*

(*a*) *The root vertex $\boldsymbol{r}$ of $H_{n,k}$ has degree*

$$\delta(\boldsymbol{r}) = \frac{(n-1)^{k+1} - (n-1)}{n-2}.$$

(*b*) *The degree of the root vertex $\boldsymbol{r}^{\boldsymbol{\alpha}}_{k-i}$ of each of the $(n-1)n^{i-1}$ subgraphs $H^{\boldsymbol{\alpha}}_{n,k-i}$, with $i = 1, 2, \ldots, k-1$, $\boldsymbol{\alpha} = \alpha_1\alpha_2 \ldots \alpha_i \in \mathbb{Z}^i_n$, and $\alpha_i \neq 0$, is*

$$\delta(\boldsymbol{r}^{\boldsymbol{\alpha}}_{k-i}) = \frac{(n-1)^{k-i+1} - (n-1)}{n-2} + (n-2).$$

(*c*) *The degree of the* $(n-1)^k$ *peripheral vertices* $\boldsymbol{p}$ *of* $H_{n,k}$ *is*

$$\delta(\boldsymbol{p}) = n + k - 2.$$

(*d*) *The degree of the* $(n-1)^{k-i}n^{i-1}$ *peripheral vertices* $\boldsymbol{p}^{\boldsymbol{\alpha}}_{k-i}$ *of the subgraphs* $H^{\boldsymbol{\alpha}}_{n,k-i}$, *with* $i = 1, 2, \ldots, k-1$, $\boldsymbol{\alpha} = \alpha_1\alpha_2\ldots\alpha_i \in \mathbb{Z}_n^i$, *and* $\alpha_i \neq 0$, *is*

$$\delta(\boldsymbol{p}^{\boldsymbol{\alpha}}_{k-i}) = n + k - i - 2.$$

Proof. (*a*) By the adjacency conditions (3) and (4), the root of $H_{n,k}$ has degree

$$\delta(\boldsymbol{r}) = \sum_{i=1}^{k}(n-1)^i = \frac{(n-1)^{k+1}-(n-1)}{n-2}.$$

(*b*) The root of the subgraph $H^{\boldsymbol{\alpha}}_{n,k-i}$, for $i = 1, 2, \ldots, k-1$, $\boldsymbol{\alpha} = \alpha_1\alpha_2\ldots\alpha_i \in \mathbb{Z}_n^i$ and $\alpha_i \neq 0$, is adjacent, by (*a*), to $\frac{(n-1)^{k-i+1}-n+1}{n-2}$ vertices belonging to the same subgraph, and also, by (5), to the $n-2$ other roots 'at the same level'.

(*c*) Each peripheral vertex of $H_{n,k}$ is adjacent, by (3), to $n-1$ vertices and, by (4), to $k-1$ roots of other subgraphs.

(*d*) Each peripheral vertex of $H^{\boldsymbol{\alpha}}_{n,k-i}$, for $i = 1, 2, \ldots, k-1$, $\boldsymbol{\alpha} = \alpha_1\alpha_2\ldots\alpha_i \in \mathbb{Z}_n^i$ and $\alpha_i \neq 0$, is adjacent, by (3), to $n-1$ vertices (of the subgraph isomorphic to K_n) and, by (4), to $k-i$ roots of other subgraphs. □

The above results on the degree distribution of $H_{n,k}$ are summarized in Table 1. Note that, from such a distribution, we can obtain again Proposition 2.2 since the number of edges can be computed from

$$2|E_{n,k}| = \delta(\boldsymbol{r}) + \sum_{i=1}^{k-1}(n-1)n^{i-1}\delta(\boldsymbol{r}^{\boldsymbol{\alpha}}_{k-i}) + (n-1)^k\delta(\boldsymbol{p}) + \sum_{i=1}^{k-1}(n-1)^{k-i}n^{i-1}\delta(\boldsymbol{p}^{\boldsymbol{\alpha}}_{k-i}),$$

which yields (7). Moreover, using this result, we see that, for a large dimension k, the average degree turns out to be of order

$$\overline{\delta} = \frac{2|E_{n,k}|}{|V_{n,k}|} = \frac{3n^{k+1}-4n^k-2(n-1)^{k+1}-n+2}{n^k} \sim n + 2k - 2.$$

From the degree distribution and for large k, we see that the number of vertices with a given degree z, $N_{n,k}(z)$, decreases as a power of the degree z and, therefore, the graph is scale-free [5, 10, 14]. As the degree distribution of the graph is discrete, to relate the exponent of this discrete degree distribution to the standard γ exponent of a continuous degree distribution for random scale-free networks, we use a cumulative distribution

$$P_{\text{cum}}(z) \equiv \sum_{z' \geq z} |N_{n,k}(z')|/|V_{n,k}| \sim z^{1-\gamma},$$

where z and z' are points of the discrete degree spectrum. When $z = \frac{(n-1)^{k-i+1}-n+2}{n-2}$, there are exactly $(n-1)n^{i-1}$ vertices with degree z. The number of vertices with this or a higher degree is

$$(n-1)n^{i-1} + \cdots + (n-1)n + (n-1) + 1 = 1 + (n-1)\sum_{j=0}^{i-1} n^j = n^i.$$

Then, we have $z^{1-\gamma} = n^i/n^k = n^{i-k}$. Therefore, for large k, $((n-1)^{k-i})^{1-\gamma} \sim n^{i-k}$ and

$$\gamma \sim 1 + \frac{\log n}{\log(n-1)}. \tag{10}$$

For $n = 5$ this gives the same value of γ as in the case of the hierarchical network introduced in [25]. This network can be obtained from $H_{5,k}$ by deleting the edges that join the roots of $H^j_{5,k-i}$, for $j \neq 0$, and $1 \leq i \leq k-2$. More generally, the same result given in (10) was already derived for the hierarchical network model of Noh [24].

Table 1: Degree and clustering distribution for $H_{n,k}$.

Vertex class	No. vertices	Degree	Clustering coefficient
$H_{n,k}$ root	1	$\frac{(n-1)^{k+1}-(n-1)}{n-2}$	$\frac{(n-2)^2}{(n-1)^{k+1}-2n+3}$
$H^{\boldsymbol{\alpha}}_{n,k-i}$ roots $i = 1,2,\ldots,k-1$, $\boldsymbol{\alpha} = \alpha_1\alpha_2\ldots\alpha_i \in \mathbb{Z}^i_n$, $\alpha_i \neq 0$	$(n-1)n^{i-1}$	$\frac{(n-1)^{k-i+1}-(n-1)}{n-2} + n - 2$	$\frac{(n-2)^2}{(n-1)^{k-i+1}+(n-1)^2-3n+4}$
$H_{n,k}$ peripheral	$(n-1)^k$	$n+k-2$	$\frac{(n-1)^2+(2k-3)(n-1)+2-2k}{(n+k-2)(n+k-3)}$
$H^{\boldsymbol{\alpha}}_{n,k-i}$ peripheral $i = 1,2,\ldots,k-1$, $\boldsymbol{\alpha} = \alpha_1\alpha_2\ldots\alpha_i \in \mathbb{Z}^i_n$, $\alpha_i \neq 0$	$(n-1)^{k-i}n^{i-1}$	$n+k-i-2$	$\frac{(n-1)^2+(2k-2i-3)(n-1)+2+2i-2k}{(n+k-i-2)(n+k-i-3)}$

Next we find the clustering distribution of the vertices of $H_{n,k}$. The clustering coefficient of a graph G measures its 'connectedness' and is another parameter used to characterize small-world and scale-free networks. The clustering coefficient of a vertex was introduced in [31] to quantify this concept. For each vertex $v \in V(G)$ with degree δ_v, its *clustering coefficient* $c(v)$ is defined as the fraction of the $\binom{\delta_v}{2}$ possible edges among the neighbors of v that are present in G. More precisely, if ϵ_v is the number of edges between the δ_v vertices adjacent to vertex v, its clustering coefficient is

$$c(v) = \frac{2\epsilon_v}{\delta_v(\delta_v - 1)}, \tag{11}$$

whereas the *clustering coefficient* of G, denoted by $c(G)$, is the average of $c(v)$ over all nodes v of G:

$$c(G) = \frac{1}{|V(G)|} \sum_{v \in V(G)} c(v). \tag{12}$$

Another definition of *clustering coefficient* of G was given in [23] as

$$c'(G) = \frac{3\,T(G)}{\tau(G)}, \tag{13}$$

where $\tau(G)$ and $T(G)$ are, respectively, the number of *triangles* (subgraphs isomorphic to K_3) and the number of *triples* (subgraphs isomorphic to a path on 3 vertices) of G. A triple at a vertex v is a 3-path with central vertex v. Thus the number of triples at v is

$$\tau(v) = \binom{\delta_v}{2} = \frac{\delta_v(\delta_v - 1)}{2}. \tag{14}$$

The total number of triples of G is denoted by $\tau(G) = \sum_{v \in V(G)} \tau(v)$. Using these parameters, note that the clustering coefficient of a vertex v can also be written as $c(v) = \frac{T(v)}{\tau(v)}$, where $T(v) = \binom{\delta_v}{2}$ is the number of triangles of G that contain the vertex v. From this result, we get that $c(G) = c'(G)$ if and only if

$$|V(G)| = \frac{\sum_{v \in V(G)} \tau(v)}{\sum_{v \in V(G)} T(v)} \sum_{v \in V(G)} \frac{T(v)}{\tau(v)}.$$

This is true for regular graphs or for graphs such that all their vertices have the same clustering coefficient. In fact, $c'(G)$ was already known in the context of social networks as *transitivity coefficient*.

We first compute the clustering coefficient and, then, the transitivity coefficient.

Proposition 4.2 *The clustering distribution of $H_{n,k}$ is the following:*

(*a*) *The root $\boldsymbol{r}$ of $H_{n,k}$ has clustering coefficient*

$$c(\boldsymbol{r}) = \frac{(n-2)^2}{(n-1)^{k+1} - 2n + 3}.$$

(*b*) *The clustering coefficient of the root vertex* $\boldsymbol{r}_{k-i}^{\boldsymbol{\alpha}}$ *of each of the* $(n-1)n^{i-1}$ *subgraphs* $H_{n,k-i}^{\boldsymbol{\alpha}}$, *with* $i = 1, 2, \ldots, k-1$, $\boldsymbol{\alpha} = \alpha_1\alpha_2\ldots\alpha_i \in \mathbb{Z}_n^i$, *and* $\alpha_i \neq 0$, *is*

$$c(\boldsymbol{r}_{k-i}^{\boldsymbol{\alpha}}) = \frac{(n-2)^2}{(n-1)n^{k-i+1} + (n-1)^2 - 3n + 4}.$$

(*c*) *The clustering coefficient of the* $(n-1)^k$ *peripheral vertices* $\boldsymbol{p}$ *of* $H_{n,k}$ *is*

$$c(\boldsymbol{p}) = \frac{(n-1)^2 + (2k-3)(n-1) + 2 - 2k}{(n+k-2)(n+k-3)}.$$

(*d*) *The clustering coefficient of the* $(n-1)^{k-i}n^{i-1}$ *peripheral vertices* $\boldsymbol{p}_{k-i}^{\boldsymbol{\alpha}}$ *of the subgraphs* $H_{n,k-i}^{\boldsymbol{\alpha}}$, *with* $i = 1, 2, \ldots, k-1$, $\boldsymbol{\alpha} = \alpha_1\alpha_2\ldots\alpha_i \in \mathbb{Z}_n^i$, *and* $\alpha_i \neq 0$ *is*

$$c(\boldsymbol{p}_{k-i}^{\boldsymbol{\alpha}}) = \frac{(n-1)^2 + (2k-2i-3)(n-1) + 2 + 2i - 2k}{(n+k-i-2)(n+k-i-3)}.$$

Proof. We prove only three of the cases, as the proof of the other is similar.

(*a*) As the root of $H_{n,k}$ is adjacent to $\sum_{i=1}^{k}(n-1)^i$ vertices with degree $n-2$, its clustering coefficient is

$$c(\boldsymbol{r}) = \frac{\frac{n-2}{2}\frac{(n-1)^{k+1}-n+1}{n-2}}{\frac{1}{2}\frac{(n-1)^{k+1}-n+1}{n-2}\left(\frac{(n-1)^{k+1}-n+1}{n-2} - 1\right)} = \frac{(n-2)^2}{(n-1)^{k+1} - 2n + 3}.$$

(*b*) The roots of $H_{n,k-i}^{\boldsymbol{\alpha}}$ ($i = 1, 2, \ldots, k-1$, and $\alpha_i \neq 0$) have clustering coefficient

$$\begin{aligned} c(\boldsymbol{r}_{k-i}^{\boldsymbol{\alpha}}) &= \frac{\frac{n-2}{2}\frac{(n-1)^{k-i+1}-n+1}{n-2} + \frac{(n-2)(n-3)}{2}}{\frac{1}{2}\left(\frac{(n-1)^{k-i+1}-n+1}{n-2} + n - 2\right)\left(\frac{(n-1)^{k-i+1}-n+1}{n-2} + n - 3\right)} \\ &= \frac{(n-2)^2}{(n-1)^{k-i+1} + (n-1)^2 - 3n + 4}. \end{aligned}$$

(*d*) The clustering coefficient of the peripheral vertices of $H_{n,k-i}^{\boldsymbol{\alpha}}$ ($i = 1, 2, \ldots, k-1$, and $\alpha_i \neq 0$) is

$$\begin{aligned} c(\boldsymbol{p}_{k-i}^{\boldsymbol{\alpha}}) &= \frac{\frac{(n-1)(n-2)}{2} + (n-2)(k-i-1)}{\frac{1}{2}(n+k-i-2)(n+k-i-3)} \\ &= \frac{(n-1)^2 + (2k-2i-3)(n-1) + 2 + 2i - 2k}{(n+k-i-2)(n+k-i-3)}. \end{aligned}$$

In particular, note that, for $i = k-1$, the peripheral vertices of $H_{n,1}^{\alpha}$, with $\alpha \neq 0$, have clustering coefficient $\frac{(n-1)^2-n+1}{(n-1)n} = 1$.

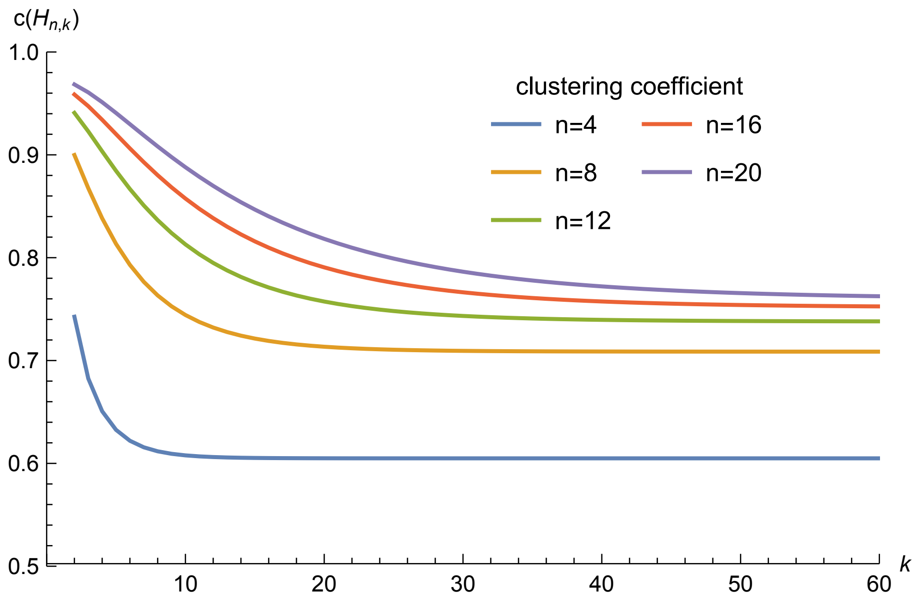

Figure 2: The clustering coefficient of $H_{n,k}$ for $n = 4, 8, \ldots, 20$.

□

The above results on the clustering distribution are summarized in Table 1. From these results, we can compute the clustering coefficient of $H_{n,k}$, which is shown in Fig. 2. The clustering coefficient tends to 1 for large n.

We think that this constant value for the clustering coefficient, which is independent of the order of the graph, together with the γ value of the power-law distribution of the degrees, is also a good characterization of *modular* hierarchical networks. Observations in metabolic networks of different organisms show that they are highly modular and have these properties, confirming the claim, see [6, 26].

To find the transitivity coefficient, we need to calculate the number of triangles and the number of triples of the graph.

Proposition 4.3 *The number $T_{n,k}$ of triangles of $H_{n,k}$ is*

$$T_{n,k} = \frac{1}{2}(n-2)\left(1 - \frac{n}{3} - (n-1)^{k+1} + \frac{2}{3}n^k(2n-3)\right).$$

Proof. When constructing $H_{n,k}$ from n copies of $H_{n,k-1}$, the adjacencies (1) and (2) introduce $(n-1)^{k-1}\binom{n-1}{2}$ and $\binom{n-1}{3}$ new triangles, respectively. Therefore,

$$T_{n,k} = nT_{n,k-1} + (n-1)^{k-1}\binom{n-1}{2} + \binom{n-1}{3}.$$

By applying recursively this formula and taking into account that $T_{n,1} = \binom{n}{3}$, we get the result. □

Moreover, from the results of Proposition 4.1 (or Table 1) giving the number of vertices of each degree, we have the following result for the number of triples (we omit the obtained explicit formula, because of its length):

Proposition 4.4 *The number $\tau_{n,k}$ of triples of $H_{n,k}$ is*

$$\tau_{n,k} = \binom{\delta(\boldsymbol{r})}{2} + (n-1)\sum_{i=1}^{k-1} n^{i-1}\binom{\delta(\boldsymbol{r}^{\boldsymbol{\alpha}}_{k-i})}{2} + (n-1)^k\binom{\delta(\boldsymbol{p})}{2} + \sum_{i=1}^{k-1}(n-1)^{k-i}n^{i-1}\binom{\delta(\boldsymbol{p}^{\boldsymbol{\alpha}}_{k-i})}{2}.$$

Now the transitivity coefficient follows from the two previous results and, as Fig. 3 shows, tends quickly to zero as $k \to \infty$. More precisely, note that the logarithmic scale shows the exponential decreasing rate.

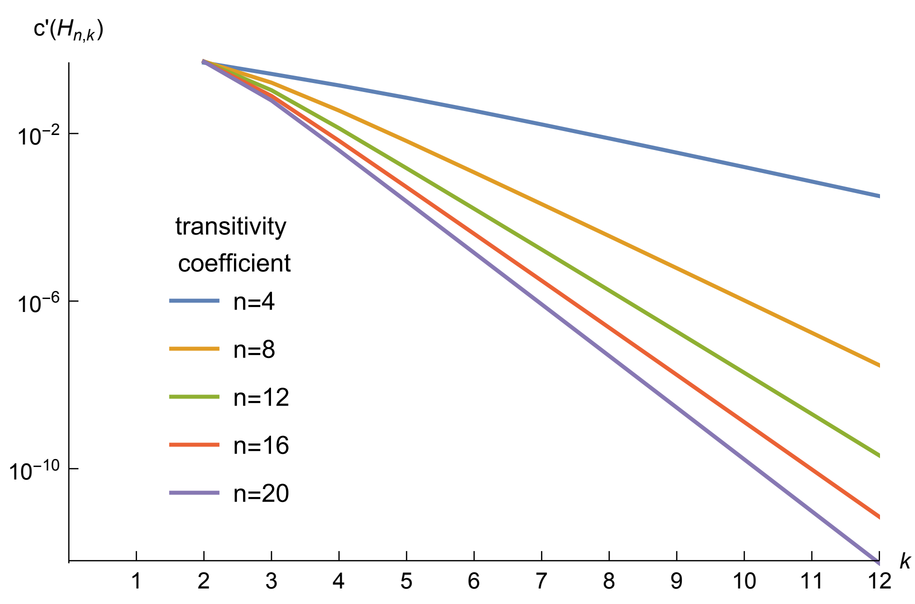

Figure 3: Transitivity coefficient of $H_{n,k}$ for $n = 4, 8, \ldots, 20$.

5 Conclusions

In this paper we have provided a family of graphs that generalize the hierarchical network introduced in [26], and combine a modular structure with a scale-free topology, in order to model modular structures associated to living organisms, social organizations and technical systems. For the proposed graphs, we have calculated their radius, diameter, degree distribution and clustering coefficient. Moreover, we have seen that they are scale-free with a power law exponent, which depends on the initial complete graph; that the clustering distribution $c(z)$ scales with the degree as z^{-1}; and that the clustering coefficient does not depend on the order of the graph, as in many networks associated to real systems [6, 25, 26]. Finally, it is worth mentioning that our definition can be generalized by taking the vertex set $\mathbb{Z}_{n_1} \times \mathbb{Z}_{n_2} \times \cdots \times \mathbb{Z}_{n_p}$ (instead of $\mathbb{Z}_n^p$), so obtaining similar results, as shown in [11].

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