Modeling complex networks with self-similar outerplanar unclustered graphs. ☆

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Abstract

This paper introduces a family of modular, self-similar, small-world graphs with clustering zero. Relevant properties of this family are comparable to those of some networks associated with technological systems with a low clustering, like the power grid or some electronic circuits. Moreover, the graphs are outerplanar and it is know that many algorithms that are NP-complete for general graphs perform polynomial in outerplanar graphs. Therefore the graphs constitute a good mathematical model for these systems.

Key words: complex networks, self-similar graphs, modular graphs, outerplanar graphs.

1. Introduction

The study, in recent years, of networks associated with complex systems has lead to the construction of models to explore their relevant properties. The first main characteristic, described by Watts and Strogatz in the paper which renewed the interest in the study of complex networks [1], is that many

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real life networks have a relatively small average distance and diameter, comparable to that of random networks with a similar number of nodes and links. In some cases the networks have also a relatively large local clustering (nodes have many mutual neighbors). However, relevant networks, like the power grid and several networks related to electronic circuits, have a very small clustering. Another important characteristic is the degree distribution. Many networks associated with social, technical and biological complex systems, like the network of citations, Internet, the WWW, protein-protein interaction network, etc., are scale-free as their degrees follow a power law [2]. This property has been considered an important signature for complex systems, but there are recent critical voices with regard to the relevance that some authors give to scale-free networks. For example, Fox-Keller [3] says that the topology of a network does not necessarily provides information about its performance in the context where it is functional and Doyle relativizes also the "universality" of scale-free networks as this topology would appear quite often associated to an optimization process when there are restrictions in its evolution, see for example [4]. Moreover, we can find many important examples of networks with degree distributions which does not follow a power law, in most cases associated with geographical or topological constraints. These systems have been modeled with networks that have exponential distributions [5] and in some cases they are also outerplanar [6, 7, 8, 9, 10] (a planar graph is called outerplanar if it has an embedding where all vertices lie on the boundary of the exterior face [11]). The original Watts and Strogatz small world network model follows also an exponential degree distribution.

The introduction of new measuring techniques allows the characterization of many real networks as self-similar and fractal [12, 13, 14]. These networks are very often hierarchical, as they describe the modularity of the systems which they model. Deterministic models for simple hierarchical networks have been published in [15, 16]. They are based on the recursive union of several basic structures to a selected root vertex. Hierarchical modularity appears also in models where the graph is constructed by adding, at each step, one or more vertices and each one is connected independently to a certain subgraph [17, 18, 19] or they are all connected together as a single structure to this given subgraph [20, 21]. The formal definition of the so-called *hierarchical product of graphs* in [22] allows a generalization and a rigorous study of some of the models.

Here, we provide a constructive algorithm to generate graphs which are outerplanar, modular and self-similar with the small-world property. It is

known that many algorithms that are NP-complete for general graphs perform polynomial in outerplanar graphs, see [23] and the related website [24]. Therefore, this family of graphs is a good mathematical model for these systems and could contribute to the development of new algorithms for complex networks.

2. Generation of the graph $M(t)$

In this section we introduce a family of modular, self-similar and outerplanar graphs which have the small-world property. We provide an iterative algorithm, and also a recursive method, for its construction. The construction method itself allows an easy determination of the order and size of the graph.

Iterative construction.– We give here an iterative formal definition of the proposed family of graphs, $M(t)$, characterized by $t \geq 0$, the number of iterations.

First, we call *generating edge* the only edge of $M(0)$ and all edges of $M(t)$ whose endvertices have been introduced at different iteration steps t. All other edges of $M(t)$ will be known as *passive edges*. A generating edge becomes passive after its use in the construction.

The graph $M(t)$ is constructed as follows:

For $t = 0$, $M(0)$ has two vertices and a generating edge connecting them.

For $t \geq 1$, $M(t)$ is obtained from $M(t-1)$ by adding to every generating edge in $M(t-1)$ a path of length three, P_4, by identifying the two final vertices of the path with the endvertices of the generating edge.

The process is repeated until the desired graph order is reached, see Fig. 1.

Recursive modular construction.– The graph $M(t)$ can be also defined as follows:

For $t = 0$, $M(0)$ has two vertices and a generating edge connecting them.

For $t = 1$, $M(1)$ is obtained from $M(0)$ by adding to its only edge a path of length three, P_4, and identifying the two final vertices of the path with the endvertices of this initial edge. Therefore $M(1)$ is a cycle of length four, C_4.

For $t \geq 2$, $M(t)$ is made from two copies of $M(t-1)$, by identifying, vertex to vertex, the initial edge of each $M(t-1)$ with two opposite edges of C_4, see Fig. 1.
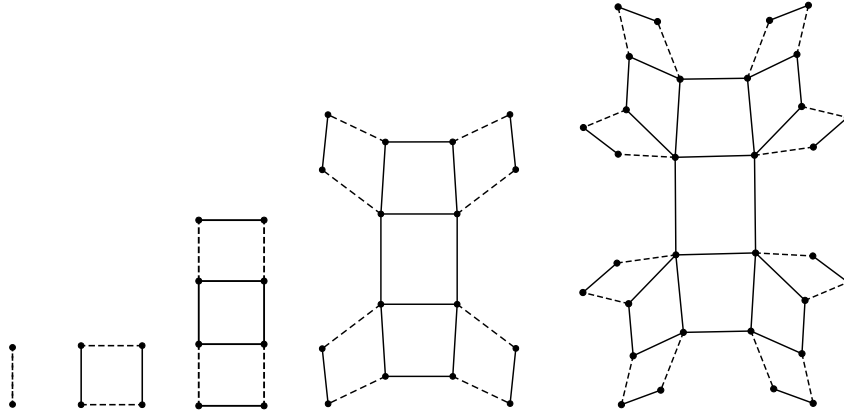
Figure 1: Graphs $M(t)$ produced at iterations $t = 0, 1, 2, 3$ and 4. Active edges are represented using dashed lines. Notice that this graph representation shows the outerplanarity of the graphs, as all the vertices lie always in the exterior face while the edges never cross.

Order and size of $M(t)$.– We use the following notation: $\tilde{V}(t)$, $\tilde{E}(t)$ and $\tilde{E}_g(t)$ denote, respectively, the set of vertices, edges and generating edges introduced at step t, while $V(t)$ and $E(t)$ denote the set of vertices and edges of the graph $M(t)$.

Notice that, at each iteration, a generating edge is replaced by two new generating edges and a passive edge. Therefore: $|\tilde{E}_g(t+1)| = 2 \cdot |\tilde{E}_g(t)|$, and $|\tilde{E}_g(t)| = 2^t$. As each generating edge introduces at the next iteration two new vertices and three new edges we have $|\tilde{V}(t+1)| = 2 \cdot |\tilde{E}_g(t)| = 2^{t+1}$ and $|\tilde{E}(t+1)| = 3 \cdot |\tilde{E}_g(t)| = 3 \cdot 2^t$. As $|\tilde{V}(0)| = 2$ and $|\tilde{E}_g(0)| = 1$, the order and size of $M(t)$, $t \geq 0$, is:

$$|V(t)| = \sum_{i=0}^{t} |\tilde{V}(i)| = 2^{t+1}, \qquad |E(t)| = \sum_{i=0}^{t} |\tilde{E}(i)| = 3 \cdot 2^t - 2. \qquad (1)$$

Planarity and outerplanarity.– A graph is planar if it can be drawn on the plane with no edges crossing. A planar graph is called outerplanar if it has an embedding in the plane such that the vertices are on a ring and the edges are drawn inside without any intersection. By construction of $M(t)$, the introduction at each iteration of a path connected to a generating edge, which afterwards becomes passive, adds two new vertices to the graph and they can be put at the exterior face with no crossing edges, see Fig. 1. The new generating edges will also lie in this exterior face keeping the outerplanarity of the graph.

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As it has been stated in the introduction, outerplanarity is an important feature for its relation to the development of efficient algorithms.

3. Topological properties of $M(t)$

Thanks to the deterministic nature of the graphs $M(t)$, we can give exact values for the relevant topological properties of this graph family, namely, degree distribution, degree correlations, diameter and average distance.

Degree distribution.– Initially, at $t = 0$, the graph has two vertices of degree one. When a new vertex i is added to the graph at iteration t_i, this vertex has degree 2 and it is connected to only one generating edge. From the construction process, every vertex of a generating edge, in the next step increases its degree in one unity and becomes the endvertex of a new generating edge.

Therefore, if we denote as $k(i,t)$ the degree of vertex i at step t, $1 \leq t_i \leq t$, we have:

$$k(i, t) = 2 + t - t_i. \tag{2}$$

The total of vertices that have been introduced at step t_i is $|\tilde{V}(t_i)| = 2^{t_i}$ and all them will have the same degree $k(i,t) = 2 + t - t_i$ at step t. Thus, by denoting as $V(t,k)$ the set of vertices that have degree k at step t, we obtain $|V(t,k)| = 2^{2+t-k}$, $2 \leq k \leq t$. Note that the two vertices introduced at steps 0 and 1 will have degree $1 + t$ at step t. Thus, $|V(t, t+1)| = 2 + 2 = 4$ for $t \geq 1$ and $|V(0,1)| = 2$.

We use the technique described by Newman in [26] to find the cumulative degree distribution $P_{\text{cum}}(k)$,

$$P_{\text{cum}}(k) = \frac{\sum_{k'=k}^{t+1} |V(t,k')|}{|V(t)|} = \frac{\sum_{k'=k}^{t} 2^{2+t-k'} + 4}{2^{t+1}} = 2^{2-k} \tag{3}$$

and therefore the degree distribution is exponential.

Some small-world networks, including the Watts-Strogatz model, have exponential degree distributions [5]. Research on networks associated to electronic circuits show that many of them are almost planar, modular and have a small clustering coefficient and in some cases their degree distributions can be associated to exponentials [25, 26].

Correlation coefficient.– We obtain here the Pearson correlation coefficient, $r(t)$, for the degrees of the endvertices of the edges of $M(t)$ [27].

$$r(t) = \frac{|E(t)| \sum_i j_i k_i - [\sum_i \frac{1}{2}(j_i + k_i)]^2}{|E(t)| \sum_i \frac{1}{2}(j_i^2 + k_i^2) - [\sum_i \frac{1}{2}(j_i + k_i)]^2} \tag{4}$$

where j_i, k_i are the degrees of the endvertices of the ith edge, with $i = 1, \cdots, |E(t)|$.

To calculate $r(t)$ we look at the degree distribution of the endvertices of all the edges of $M(t)$ at a given step t_i.

At this step t_i, $t_i \geq 2$, 2^{t_i-1} new passive edges are added to the graph and all their endvertices have the same degree 2. Each new iteration will increase the degree of these vertices in one unity. Therefore, at step t, the vertices will have degree $k = 2 + t - t_i$. As $2 \leq t_i \leq t$, we note that there are 2^{1+t-k} edges which join vertices with degree k, $2 \leq k \leq t$.

At this same iteration step t_i, 2^{t_i} new generating edges are introduced to the graph. These edges connect the new vertices, which have degree 2, to every vertex of $M(t_i - 1)$ which has the following degree distribution at step $t_i - 1$: $|V(t_i - 1, l - 1)| = 2^{2+t_i-l}$, $3 \leq l \leq t_i$, and $|V(t_i - 1, t_i)| = 4$. At each step all these vertices will increase their degree in one unity.

If we denote by $\langle j, k \rangle$ an edge connecting vertices of degrees j and k, we find, at step t_i and for $3 \leq l \leq t_i$, the following distribution of new generating edges: 2^{2+t_i-l} edges $\langle 2, l \rangle$, and four edges $\langle 2, t_i + 1 \rangle$. At step t, $3 \leq l \leq t_i \leq t$, the distribution is: 2^{2+t_i-l} edges $\langle 2 + t - t_i, l + t - t_i \rangle$ and 4 edges $\langle 2 + t - t_i, 1 + t \rangle$.

Note that the four edges introduced at steps 0 and 1, whose endvertices have degree 2 at step 1, will have degree $t + 1$ at step t, $t \geq 2$.

Table 1 displays a summary of the results. The upper part corresponds to passive edges, the middle part to generating edges and the last row to the four edges introduced at steps 0 and 1.

Using this analysis, we can find the sums of Eq. 3:

$$\sum_i j_i k_i = \sum_{l=2}^{t} 2^{1+t-l} l^2 + 4 \sum_{l=2}^{t+1} (t+1)l + \sum_{k=3}^{t} \sum_{l=2}^{k-1} 2^{2+t-k} k\, l$$
$$= -4t^2 - 26t - 44 + 45 \cdot 2^t,$$

$$\sum_i (j_i + k_i) = \sum_{l=2}^{t} 2^{1+t-l} 2l + 4 \sum_{l=2}^{t+1} (t+1+l) + \sum_{k=3}^{t} \sum_{l=2}^{k-1} 2^{2+t-k} (k+l)$$

Degree of vertex i	Degree of vertex j	Number of edges
t	t	2
$t-1$	$t-1$	2^2
$\vdots$	$\vdots$	$\vdots$
l	l	2^{1+t-l}
$\vdots$	$\vdots$	$\vdots$
2	2	2^{t-1}
$t+1$	t	4
$t+1$	$t-1$	4
$\vdots$	$\vdots$	$\vdots$
$t+1$	2	4
t	$t-1$	2^2
t	$t-2$	2^2
$\vdots$	$\vdots$	$\vdots$
t	2	2^2
$\vdots$	$\vdots$	$\vdots$
l	$l-1$	2^{2+t-l}
l	$l-2$	2^{2+t-l}
$\vdots$	$\vdots$	$\vdots$
l	2	2^{2+t-l}
$\vdots$	$\vdots$	$\vdots$
3	2	2^{2+t-3}
$t+1$	$t+1$	4

Table 1: Number of edges in $M(t)$ according to the degrees of their endvertices.

$$= -8t + 22 \cdot 2^t - 20,$$

$$\sum_i (j_i^2 + k_i^2) = \sum_{l=2}^{t} 2^{1+t-l} 2l^2 + 4\sum_{l=2}^{t+1}((t+1)^2 + l^2) + \sum_{k=3}^{t}\sum_{l=2}^{k-1} 2^{2+t-k}(k^2 + l^2)$$

$$= -12t^2 - 60t + 102 \cdot 2^t - 100.$$

Finally, we obtain the correlation coefficient as:

$$r(t) = \frac{12 \cdot 2^t t^2 - 10 \cdot 2^t t + 2^{1+t} - 14 \cdot 4^t + 8t^2 + 28t + 12}{18 \cdot 2^t t^2 + 2^{1+t}t - 32 \cdot 4^t + 32 \cdot 2^t + 4 \cdot t^2 + 20t}. \tag{5}$$

Notice that, for large values of t, $r(t) \sim \frac{7}{16} = 0.4375$. Therefore this family of graphs has the degrees of the endvertices positively correlated and the graph is assortative. Social networks are usually assortative as it is also the case of some technical networks like the power grid and electronic circuits, see [27, 28].

Diameter.– At each iteration step we introduce, for every generating edge, two new vertices which are adjacent. As each vertex joins the graph of the former step through one new edge, the diameter will increase by exactly 2 units. Therefore $D(t) = D(t-1) + 2$, $t \geq 2$. As $D(1) = 2$, we have that the diameter of $M(t)$ is $D(t) = 2 \cdot t$, $t \geq 1$. Therefore, from Eq. 1, and as for t large, $t \sim \ln |V_t|$ we have in this limit that $D_t \propto \ln |V_t|$.

Average distance.– The average distance of $M(t)$ is defined as:

$$\bar{d}_t = \frac{1}{|V(t)|(|V(t)| - 1)/2} \sum_{i,j \in V(t)} d_{i,j}, \tag{6}$$

where $d_{i,j}$ is the distance between vertices i and j. In what follows, $S(t)$ will denote the sum $\sum_{i,j \in V(t)} d_{i,j}$.

We use the modular recursive construction of $M(t)$ to obtain the exact value of $\bar{d}_t$. The graph $M(t+1)$ is obtained from the juxtaposition of two copies of $M(t)$, $M_1(t)$ and $M_2(t)$, on top of the cycle C_4, see Figs. 1 and 2.

The two copies $M_1(t)$ and $M_2(t)$ are connected one to another at *connecting vertices* $\{X, Y\}$ in $M_1(t)$ and $\{Z, O\}$ in $M_2(t)$. All other vertices of the graph $M(t+1)$ will be called *interior vertices*.

Let $\Delta_t^{1,2}$ denote the sum of all shortest paths between interior vertices from $M_1(t)$ to $M_2(t)$. We also denote by Δ_t de sum of all distances from the
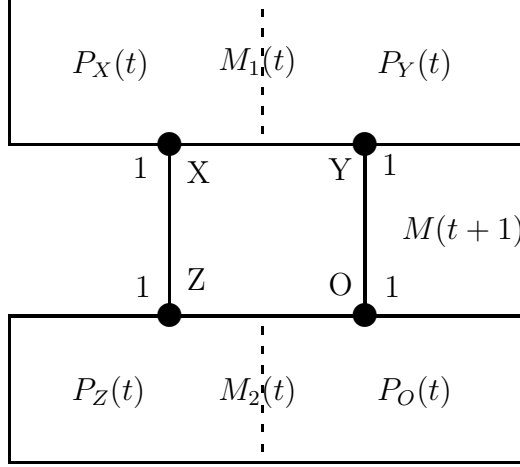
Figure 2: Two copies of the graph $M(t)$, $M_1(t)$ and $M_2(t)$, are joined through connecting vertices X, Y, Z and O to form the graph $M(t+1)$.

interior vertices of $M_1(t)$ and $M_2(t)$ to the connecting vertices of the other copy.

The sum of all distances in $M(t+1)$, $S(t+1)$, satisfies:

$$S(t+1) = 2S(t) + \Delta_t^{1,2} + \Delta_t. \tag{7}$$

Now, we classify the interior vertices of the graph $M_1(t)$ into two different classes, $P_X(t)$ and $P_Y(t)$, according to their shortest path lengths to each of the two vertices $\{X, Y\}$. In the same way are classified the interior vertices of $M_2(t)$ into $P_Z(t)$ and $P_O(t)$. From the symmetry in the graph,

$$|P_X(t)| = |P_Y(t)| = |P_Z(t)| = |P_O(t)| = \frac{|M(t)| - 2}{2} = 2^t - 1$$

, and

$$\sum_{i \in P_X(t)} d_{X,i} = \sum_{i \in P_Y(t)} d_{Y,i} = \sum_{i \in P_Z(t)} d_{Z,i} = \sum_{i \in P_O(t)} d_{O,i} = 2^{t-1}t. \tag{8}$$

We have:

$$\Delta_t = \sum_{i \in V_2(t)\setminus\{Z,O\}} d_{X,i} + \sum_{i \in V_2(t)\setminus\{Z,O\}} d_{Y,i} +$$

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$$+ \sum_{i \in V_1(t)\backslash\{X,Y\}} d_{Z,i} + \sum_{i \in V_1(t)\backslash\{X,Y\}} d_{O,i} + 6 =$$

$$= 4 \sum_{i \in V_2(t)\backslash\{Z,O\}} d_{X,i} + 6 = 4 \left(\sum_{i \in P_Z(t)} d_{X,i} + \sum_{i \in P_O(t)} d_{X,i} \right) + 6 =$$

$$= 4 \left(\sum_{i \in P_Z(t)} (d_{X,Z} + d_{Z,i}) + \sum_{i \in P_O(t)} (d_{X,O} + d_{O,i}) \right) + 6 =$$

$$= 4 \left(|P_Z(t)| + 2^{t-1}t + 2|P_O(t)| + 2^{t-1}t \right) + 6 =$$

$$= 4(2 \cdot 2^{t-1}t + 3(2^t - 1)) + 6 = 2^{t+2}(t+3) - 6. \tag{9}$$

On the other hand, to calculate $\Delta_t^{1,2}$, we find:

$$\sum_{u \in P_X(t), v \in P_Z(t)} d_{u,v} = \sum_{u \in P_X(t)} \sum_{v \in P_Z(t)} d_{u,v} = \sum_{u \in P_X(t)} \sum_{v \in P_Z(t)} (d_{u,X} + d_{X,Z} + d_{Z,v}) =$$

$$= \sum_{u \in P_X(t)} \left(\sum_{v \in P_Z(t)} d_{u,X} + \sum_{v \in P_Z(t)} d_{X,Z} + \sum_{v \in P_Z(t)} d_{Z,v} \right) =$$

$$= \sum_{u \in P_X(t)} \left(|P_Z(t)| d_{u,X} + |P_Z(t)| + 2^{t-1}t \right) =$$

$$= |P_Z(t)| 2^{t-1}t + |P_Z(t)||P_X(t)| + |P_X(t)| 2^{t-1}t$$

$$= 2(2^t - 1) 2^{t-1}t + (2^t - 1)^2.$$

Analogously,

$$\sum_{u \in P_X(t), v \in P_O(t)} d_{u,v} = 2(2^t - 1) 2^{t-1}t + 2(2^t - 1)^2.$$

Therefore, using again the symmetry of the graph, we have:

$$\Delta_t^{1,2} = 8(2^t - 1)2^{t-1}t + 6(2^t - 1)^2 = (2^t - 1)2^{t+2}t + 6(2^t - 1)^2. \tag{10}$$

From (7), (9) and (10), we obtain the recursive expression for the total distance $S(t+1)$:

$$S(t+1) = 2S(t) + (2^t - 1)2^{t+2}t + 6(2^t - 1)^2 + 2^{t+2}(t+3) - 6. \tag{11}$$

We solve this equation inductively, using the initial condition S(1)=8, and we have

$$S(t) = 2^{t+1} + 4^t(2t - 1). \tag{12}$$

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Finally, the average distance of $M(t)$ results

$$\overline{d}(t) = \frac{2^{t+1} + 4^t(2t-1)}{|V(t)|(|V(t)|-1)/2} = \frac{2 + 2^t(2t-1)}{2^{t+1} - 1}. \tag{13}$$

Notice that for a large iteration step, $t \to \infty$, $\overline{d}_t \simeq t \sim \ln|V_t|$, which shows a logarithmic scaling of the average distance with the order of the graph. As we have found a similar behavior for the diameter, the graph is small-world.

4. Conclusion

We have introduced and studied a family of graphs which are planar, modular, have a degree hierarchy and are also small-world. At the same time the graphs have clustering zero. A combination of modularity, small clustering coefficient, and small-world properties can be found in real networks like some social and technical networks [26, 25]. Therefore this model, with a null clustering coefficient, can be considered to model these networks and also it can be used to study other properties with independence of the clustering. On the other hand, the graphs are outerplanar and it is known that many algorithms that are NP-complete for general graphs perform polynomial in outerplanar graphs. This should be useful to find new efficient algorithms for complex networks Finally, the deterministic character of the family, as opposed to usual probabilistic models, should facilitate the exact computation of other network parameters.

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