Computing the Wiener index in Sierpiński carpet graphs

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Abstract. We describe an algorithm to compute the Wiener index of a sequence of finite graphs approximating the Sierpiński carpet.

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INTRODUCTION

The famous Sierpiński carpet is a self-similar, infinitely ramified fractal introduced by W. Sierpiński in 1916 [12]. Many physical models and critical phenomena on this and other related fractals, or on their discrete approximations, have been widely studied in the literature [1, 4, 5, 9, 10, 11]. In this short note, we study the Wiener index of a sequence \( \{ \Gamma_n \} \) of graphs defined below.

WIENER INDEX AND CARPET GRAPHS

Let \( \Gamma = (V, E) \) be a connected finite graph. The Wiener index \( W(\Gamma) \) of \( \Gamma \) is the number

\[
W(\Gamma) = \frac{1}{2} \sum_{v \neq w \in V} d(v, w),
\]

where \( d \) is the geodesic distance on \( \Gamma \). We investigate it for the sequence of \( \Gamma_n \) defined below.

Fix two finite alphabets \( X = \{0, 1, \ldots, 7\} \) and \( Y = \{a, b, c, d\} \), and let \( X^n = \{x_1, x_2, \ldots : x_i \in X\} \) be the set of all infinite words over \( X \). Let \( C_4 \) be the cyclic graph of length 4 whose vertices will be denoted by \( a, b, c, d \) (Fig. 1).

Recursive construction of the graphs \( \Gamma_n \).

• Step 1. The graph \( \Gamma_1 \) is the cyclic graph \( C_4 \).

• Step \( n - 1 \to n \). Take 8 copies of \( \Gamma_{n-1} \) and glue them together on the model graph \( \overline{\Gamma} \), in such a way that these copies occupy the positions indexed by 0, 1, \ldots, 7 in \( \Gamma \) (Fig. 1). Note that each copy shares at most one (extremal) side with any other copy. A vertex of \( \Gamma_n \) is associated with the word \( yx_1 \ldots x_{n-1} \in Y \times X^{n-1} \), if it belongs to the copy of \( \Gamma_{n-1} \) indexed by \( x_{n-1} \) contained in \( \Gamma_n \), and if it was associated with the word \( yx_1 \ldots x_{n-2} \) at the previous step. Notice that any word in \( Y \times X^{n-1} \) corresponds to a unique vertex of \( \Gamma_n \), but the viceversa is not true.

In Fig. 1, for instance, the vertex associated with the word \( c45 \) in \( \Gamma_3 \) also corresponds to the word \( d64 \).
The graph $\Gamma_n$ can be embedded into $\mathbb{Z}^2$, in such a way that the left corner vertex on the bottom of $\Gamma_n$ coincides with the vertex $(0,0)$ of $\mathbb{Z}^2$, and each horizontal edge of $\Gamma_n$ coincides with an edge of $\mathbb{Z}^2$ connecting two vertices of type $v$ and $v \pm (1,0)$, whereas each vertical edge of $\Gamma_n$ coincides with an edge of $\mathbb{Z}^2$ connecting two vertices of type $w$ and $w \pm (0,1)$. This embedding does not preserve, in general, the distances. In fact, the bigger and bigger holes, denoted by $H_n$, that we produce in our recursive construction may contain edges that belong to the shortest path connecting two vertices of $\Gamma_n$ after its embedding into $\mathbb{Z}^2$. In some sense, these holes correspond to obstructions (in the terminology of [3]) that should be taken into account in order to determine $W(\Gamma_n)$. In what follows, we analyse all possible cases in which the distances between vertices differ from the case $\mathbb{Z}^2$: we will say that the path joining such vertices meets an obstruction. The representation of the vertices of $\Gamma_n$ in terms of words in $Y \times X^{n-1}$, the description of the obstructions and the symmetry of the graphs $\Gamma_n$ allow us to describe an algorithm to compute $W(\Gamma_n)$.

In order to explicitly describe the embedding of $\Gamma_n$ into $\mathbb{Z}^2$, we define the following vectors of $\mathbb{Z}^2$ associated with the letters of the alphabet $Y$:

$$v_0 = (0,0) \quad v_1 = (1,0) \quad v_2 = (1,1) \quad v_3 = (0,1)$$

and the following vectors of $\mathbb{Z}^2$ associated with the letters of the alphabet $X$:

$$v_0 = (0,0) \quad v_1 = (1,0) \quad v_2 = (2,0) \quad v_3 = (2,1) \quad v_4 = (2,2) \quad v_5 = (1,2) \quad v_6 = (0,2) \quad v_7 = (0,1)$$

Now let $w_n = yx_1x_2\ldots x_{n-1} \in Y \times X^{n-1}$; we associate with $w_n$ a vector $w_n$ of $\mathbb{Z}^2$ defined as $w_n = v_y + \sum_{i=1}^{n-1} 3^{i-1} v_{x_i}$.

Given two finite words $w_1^{1}$ and $w_2^{1}$ and the corresponding vectors $w_1^{1}(X(w_1^{1}), Y(w_1^{1}))$ and $w_2^{1}(X(w_2^{1}), Y(w_2^{1}))$, we put $\|w_1^{1} - w_2^{1}\| = |X(w_1^{1}) - X(w_2^{1})| + |Y(w_1^{1}) - Y(w_2^{1})|$, which is the geodesic distance in $\mathbb{Z}^2$. Given $w_1^{1} = y^1x_1^{1}\ldots x_{n-1}^{1}, w_2^{1} = y^2x_1^{2}\ldots x_{n-1}^{2} \in Y \times X^{n-1}$, let $h = \max_{i=1,\ldots,n-1}(i : x_{i}^{1} \neq x_{i}^{2})$. Note that if $x_{i}^{1} = x_{i}^{2}$ for each $i = 1, \ldots, n-1$, then $d(w_1^{1}, w_2^{1})$ can take the values 0, 1, 2, depending on the first letters of $w_1^{1}$ and $w_2^{1}$ (the vectors correspond to vertices belonging to the same square of side 1).

By definition of the index $h$, the distance $d(w_1^{1}, w_2^{1})$ equals the distance $d(w_{h+1}^{1}, w_{h+1}^{2})$ in the graph $\Gamma_{h+1}$; observe that the vectors $w_{h+1}^{1}$ and $w_{h+1}^{2}$ are associated with the truncated words $y^1x_1^{1}\ldots x_{h}^{1}$ and $y^2x_1^{2}\ldots x_{h}^{2}$, and they occupy two distinct copies of the graph $\Gamma_{h+1}$, indexed by $x_{h}^{1}$ and $x_{h}^{2}$, respectively.

**CASE I**: $d(w_{h+1}^{1}, w_{h+1}^{2}) = \|w_{h+1}^{1} - w_{h+1}^{2}\|$, since there is no obstruction in the shortest path from $w_{h+1}^{1}$ to $w_{h+1}^{2}$ in $\Gamma_{h+1}$. This occurs in the following cases:

- $x_{h}^{1} = 0, x_{h}^{2} = 4; x_{h}^{1} = 2, x_{h}^{2} = 6$.
- $x_{h}^{1} = 0, x_{h}^{2} = 3; x_{h}^{1} = 1, x_{h}^{2} = 4; x_{h}^{1} = 2, x_{h}^{2} = 5; x_{h}^{1} = 3, x_{h}^{2} = 6; x_{h}^{1} = 4, x_{h}^{2} = 7; x_{h}^{1} = 5, x_{h}^{2} = 0; x_{h}^{1} = 6, x_{h}^{2} = 1; x_{h}^{1} = 7, x_{h}^{2} = 2$.
- $x_{h}^{1} = 1, x_{h}^{2} = 3; x_{h}^{1} = 3, x_{h}^{2} = 5; x_{h}^{1} = 5, x_{h}^{2} = 7; x_{h}^{1} = 7, x_{h}^{2} = 1$.

**CASE II**

$x_{h}^{1} = 1, x_{h}^{2} = 5$: we have to consider two different subcases. First of all, observe that the corner vertices of middle hole
Now if \( \frac{X(w_{h+1}^1)+X(w_{h+1}^2)}{2} \geq \frac{X(A_{h+1})+X(B_{h+1})}{2} = \frac{3h}{2} \), then:
\[
d(w_{h+1}, w_{h+1}^2) = d(w_{h+1}, B_{h+1}) + d(B_{h+1}, C_{h+1}) + d(C_{h+1}, w_{h+1}^2) = \|w_{h+1}^1 - B_{h+1}\|_1 + 3^{h-1} + \|C_{h+1} - w_{h+1}^2\|_1.
\]
Similarly, if \( \frac{X(w_{h+1}^1)+X(w_{h+1}^2)}{2} < \frac{X(A_{h+1})+X(B_{h+1})}{2} = \frac{3h}{2} \), then
\[
d(w_{h+1}, w_{h+1}^2) = \|w_{h+1}^1 - A_{h+1}\|_1 + 3^{h-1} + \|D_{h+1} - w_{h+1}^2\|_1.
\]
An analogous argument holds in the case \( x_3^1 = 3, x_4^2 = 7 \).

**CASE III**

\( x_1^3 = 0, x_2^2 = 2 \). Let us put \( \ell = \max\{j : x_j^1 = 7\} \). We put \( \ell = -\infty \) if \( x_j^1 \neq 7 \), for each \( j = 1, \ldots, h - 1 \).

- **Case \( \ell = -\infty \)**. We have \( d(w_{h+1}^1, w_{h+1}^2) = \|w_{h+1}^1 - w_{h+1}^2\|_1 \), since there is no obstruction in the shortest path from \( w_{h+1}^1 \) to \( w_{h+1}^2 \) in \( \Gamma_{h+1} \).
- **Case \( \ell \neq -\infty \)**. Any geodesic path joining \( w_{h+1}^1 \) to \( w_{h+1}^2 \) in \( \Gamma_{h+1} \) meets an obstruction (the largest one) given by a hole isomorphic to \( H_{\ell+1} \), whose corner vertices are:

\[
\begin{align*}
A_{\ell+1} &= (3^{\ell+1}, 3^{\ell+1}) + \sum_{k=\ell+1}^{h} 3^{k-1} v_{x_k^1} \\
B_{\ell+1} &= (2 \cdot 3^{\ell+1}, 3^{\ell+1}) + \sum_{k=\ell+1}^{h} 3^{k-1} v_{x_k^1} \\
C_{\ell+1} &= (2 \cdot 3^{\ell+1}, 2 \cdot 3^{\ell+1}) + \sum_{k=\ell+1}^{h} 3^{k-1} v_{x_k^1} \\
D_{\ell+1} &= (3^{\ell+1}, 2 \cdot 3^{\ell+1}) + \sum_{k=\ell+1}^{h} 3^{k-1} v_{x_k^1}.
\end{align*}
\]

Now if \( \frac{Y(w_{h+1}^1)+Y(w_{h+1}^2)}{2} \geq \frac{Y(A_{\ell+1})+Y(D_{\ell+1})}{2} \), then:
\[
d(w_{h+1}, w_{h+1}^2) = d(w_{h+1}, D_{\ell+1}) + d(D_{\ell+1}, C_{\ell+1}) + d(C_{\ell+1}, w_{h+1}^2) = \|w_{h+1}^1 - D_{\ell+1}\|_1 + 3^{\ell+1} + \|C_{\ell+1} - w_{h+1}^2\|_1.
\]
Similarly, if \( \frac{Y(w_{h+1}^1)+Y(w_{h+1}^2)}{2} < \frac{Y(A_{\ell+1})+Y(D_{\ell+1})}{2} \), then
\[
d(w_{h+1}, w_{h+1}^2) = \|w_{h+1}^1 - A_{\ell+1}\|_1 + 3^{\ell+1} + \|B_{\ell+1} - w_{h+1}^2\|_1.
\]

The same argument holds in the cases \( x_3^1 = 6, x_4^2 = 4 \). Moreover, an analogous method works in the cases \( x_3^1 = 2, x_4^2 = 4 \) and \( x_3^1 = 0, x_4^2 = 6 \), but now the definition of \( \ell \) must be replaced with \( \ell' = \max\{j : x_j^1 = 1\} \), since we have now to consider the obstruction that we meet when we move from the bottom to the top of \( \Gamma_{h+1} \).

**CASE IV**

\( x_1^1 = 0, x_2^2 = 1 \). Let us define \( \ell \) as in Case III.

- **Case \( \ell = -\infty \)**. In this case, we have \( d(w_{h+1}^1, w_{h+1}^2) = \|w_{h+1}^1 - w_{h+1}^2\|_1 \), since there is no obstruction in the shortest path from \( w_{h+1}^1 \) to \( w_{h+1}^2 \) in \( \Gamma_{h+1} \).
- **Case \( \ell \neq -\infty \)**. Any geodesic path connecting \( w_{h+1}^1 \) to \( w_{h+1}^2 \) in \( \Gamma_{h+1} \) meets an obstruction (the largest one) given by a hole isomorphic to \( H_{\ell+1} \), whose corner vertices are defined as in (1). If \( \frac{Y(w_{h+1}^1)+Y(w_{h+1}^2)}{2} \geq \frac{Y(A_{\ell+1})+Y(D_{\ell+1})}{2} \), then:
\[
d(w_{h+1}, w_{h+1}^2) = d(w_{h+1}, D_{\ell+1}) + d(D_{\ell+1}, C_{\ell+1}) + d(C_{\ell+1}, w_{h+1}^2) = \|w_{h+1}^1 - D_{\ell+1}\|_1 + 3^{\ell+1} + \|C_{\ell+1} - w_{h+1}^2\|_1.
\]
Similarly, if \( \frac{Y(w_{h+1}^1)+Y(w_{h+1}^2)}{2} < \frac{Y(A_{\ell+1})+Y(D_{\ell+1})}{2} \), then
\[
d(w_{h+1}, w_{h+1}^2) = \|w_{h+1}^1 - A_{\ell+1}\|_1 + 3^{\ell+1} + \|B_{\ell+1} - w_{h+1}^2\|_1.
\]
The same argument holds in the cases \( x_3^1 = 1, x_4^2 = 2; x_3^1 = 6, x_4^2 = 5; x_3^1 = 5, x_4^2 = 4 \). Finally, a similar argument works in the cases \( x_3^1 = 0, x_4^2 = 7; x_3^1 = 7, x_4^2 = 6; x_3^1 = 2, x_4^2 = 3; x_3^1 = 3, x_4^2 = 4 \), where \( \ell \) must be replaced with the index \( \ell' \) defined as in the last part of Case III.

**Example 1.** In Fig. 2 we have represented in \( \Gamma_4 \) the vertices corresponding to the words \( w_4^1 = a670 \) and \( w_4^2 = b432 \). The corresponding vectors, after the embedding into \( \mathbb{Z}^2 \), are \( (0,5) \) and \( (27,5) \), respectively. We have \( n = 4, h = 3, \ell = 2 \), so that \( A_3(3,3), B_3(6,3), C_3(6,6), D_3(3,6) \) are the corner vertices of the first of the three biggest obstructions met by the shortest path from \( w_4^1 \) to \( w_4^2 \) (case III). One has \( d(w_4^1, w_4^2) = 29 \).
In the previous description we have redundancy if we consider all possible words in \( Y \times X^{n-1} \). In fact, as we pointed out before, different words may correspond to the same vertex of \( \Gamma_n \). We solve this problem by giving a lexicographic order to such words and considering the smallest one.

**Theorem 2.** The sum of the distances between all vertices obtained in the cases I, II, III, IV and considered without redundancy is the Wiener index \( W(\Gamma_n) \).

The numerical values of \( W(\Gamma_n) \) have been computed by using the commercial software Wolfram Mathematica and are reported in Table 1.

| \( n \) | \( 8 \) | \( 320 \) | \( 31264 \) | \( 4642456 \) |
| --- | --- | --- | --- | --- |
| 1 | | | |
| 2 | | | |
| 3 | | | |
| 4 | | | |
| 5 | | | |
| 6 | | | |

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