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Complexity of Topological Indices: The Case of Connective Eccentric Index

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Abstract Let I be a summation-type topological index and let G be a graph. The I-complexity $C_I(G)$ of G is introduced as the number of different contributions to $I(G)$ in its summation formula. The complexity is studied in the case of the connective eccentric index $\xi^{\rm ce}$. For any $d \geq 2$ and for any $k \geq 1$, a graph G with ${\rm diam}(G) = d$ and $C_{\xi^{\rm ce}}(G) = k$ is constructed. Graphs with $C_{\xi^{\rm ce}}(G) = 1$ are studied and infinite families of such graphs that are not vertex-transitive are constructed. A cut-method theorem for the vertex eccentricity is also developed.

1 Introduction

Let $\mathcal{G}$ be the class of all graphs. A function $I : \mathcal{G} \to \mathbb{R}$ which is invariant under graph isomorphisms is called a *topological index*. These indices are omnipresent in chemical graph theory and have found a variety of applications; see the books [11, 12, 24] and papers [13, 22] for appealing recent examples.

For a given graph $G = (V, E)$, a topological index I is often of the form

$$I(G) = \sum_{v \in V} f(v)\,, \tag{1}$$

where $f(v)$ is some function of the vertex v, for instance a function of its degree, of its eccentricity, and/or of its distances. For instance, if $d(v)$ denotes the sum of the distances from v to all the other vertices, then setting $f(v) = d(v)/2$, Equation (1) turns into $I(G) = W(G)$, where $W(G)$ is the celebrated Wiener index of G, see the surveys [7, 8], recent papers [10, 18, 21], and references therein.

Let now $G = (V, E)$ be a graph and let I be a topological index of the form (1). Then we say that vertices u and v of G are in relation $\sim_I$ if $f(u) = f(v)$. Clearly, $\sim_I$ is an equivalence relation. Let $V/_{\sim_I} = \{V_1, \ldots, V_k\}$ be its equivalence classes and let $v_i \in V_i$, $i \in [k] = \{1, \ldots, k\}$, be the representatives of the classes. Then

$$I(G) = \sum_{i=1}^{k} |V_i| f(v_i)\,. \tag{2}$$

We define $|V/_{\sim_I}|$ to be the *I-complexity* of G and denote it with $C_I(G)$. Hence $C_I : \mathcal{G} \to \mathbb{N}$.

The summation in (1) runs over all vertices of G. If instead a topological index is defined in view of (1) but replacing the vertex set with the edge set of a given graph (as it is also often the case, e.g. in Szeged-like indices), then we define the I-complexity analogously.

In the particular case when $I = W$, the function $C_W(G)$ was earlier studied in [1] under the name *Wiener dimension* of a graph. In the general framework proposed here we prefer to use the word "complexity" instead of "dimension" since the latter word has usually a different, geometric flavour. On the other hand, $C_I(G)$ tells how complex is the computation of I on G.

We proceed as follows. In the next section we introduce concepts and notations needed in this paper. We also demonstrate that any possible diameter d and any possible positive integer k, a graph exists with diameter d and $\xi^{\rm ce}$-complexity k. In Section 3 graphs with $\xi^{\rm ce}$-complexity equal to 1 are studied with an emphasis on graphs that are not vertex-transitive. In the final section we prove a cut-method theorem for the vertex eccentricity.

2 Preliminaries and realizability of the $\xi^{\rm ce}$-complexity

All graphs considered will be connected. A graph G is *vertex-transitive* if to any vertices u and v of G there exists an automorphism ϕ of G such that $\phi(u) = v$. The *Cartesian product* $G \,\Box\, H$ of graphs G and H has vertex set $V(G \,\Box\, H) = V(G) \times V(H)$, vertices (g, h) and (g', h') being adjacent if $g = g'$ and $hh' \in E(H)$, or $h = h'$ and $gg' \in E(G)$.

The Cartesian product graph operation is associative, hence we may consider powers of graphs with respect to it. Powers of K_2 are known as *hypercubes*, the d-tuple power is denoted with Q_d. In other words, the vertex set of Q_d consists of all binary vectors of length d, two such vectors being adjacent if they differ in exactly one coordinate.

The degree of a vertex u of a graph G is denoted with $\deg_G(u)$. The distance $d_G(u,v)$ between vertices u and v of a graph G is the number of edges on a shortest u,v-path. The *eccentricity* $\mathrm{ecc}_G(u)$ of a vertex u is $\max\{d_G(u,x):\ x \in V(G)\}$. If G is clear from the context we may (and will) omit G as a subscript in the above notations. The *radius* $\mathrm{rad}(G)$ and the *diameter* $\mathrm{diam}(G)$ are the minimum and the maximum eccentricity of its vertices, respectively. A subgraph H of a graph G is an *isometric subgraph* if $d_H(u,v) = d_G(u,v)$ holds for any vertices $u,v \in V(H)$. Isometric subgraphs of hypercubes are known as *partial cubes*. Many chemical graphs are partial cubes as for instance trees and benzenoid graphs.

The *connective eccentricity index* of a graph $G = (V,E)$ is defined as

$$\xi^{\mathrm{ce}}(G) = \sum_{v\in V} \frac{\deg(v)}{\mathrm{ecc}(v)}\,.$$

This index was introduced in [14] as a novel topological descriptor for predicting biological activity and received considerable attention afterwards, cf. [25–27]. For a comprehensive list of all eccentricity based topological indices introduced see [19]. We note in passing that the closely related *eccentric connectivity index* ξ^{c} of a graph G was introduced in [23] as $\xi^{\mathrm{c}}(G) = \sum_{v\in V} \deg(v)\mathrm{ecc}(v)$, cf. [4, 5, 9].

The unique graphs of diameter 1 are complete graphs. Clearly, $C_{\xi^{\mathrm{ce}}}(K_n) = 1$ holds for any $n \geq 1$. On the other hand, as soon as the diameter is at least 2, all ξ^{ce}-complexities are possible as the next theorem asserts. For its proof we need the following well-known fact, cf. [15, Proposition 3.1(i)].

Lemma 2.1 *If* $d \geq 1$, *then* $\mathrm{diam}(Q_d) = d$.

Theorem 2.2 *For any* $d \geq 2$ *and for any* $k \geq 1$ *there exists a graph* G *such that* $\mathrm{diam}(G) = d$ *and* $C_{\xi^{\mathrm{ce}}}(G) = k$.

Proof. For $k = 1$ and $d \geq 2$ any vertex-transitive graph of diameter d does the job. For instance, $\mathrm{diam}(C_{2d}) = d$ and $C_{\xi^{\mathrm{ce}}}(C_{2k}) = k$.

Let now $k \geq 2$, and let G_k be the graph on the vertex set $[k+1]$, where $ij \in E(G_k)$ if and only if $i + j \leq k + 2$. Note that the vertex 1 of G_k is of degree $k = |V(G_k)| - 1$. Hence, since G_k is not a complete graph, it follows that $\mathrm{diam}(G_k) = 2$. Note further that the degree sequence of G_k is

$$k, k-1, \ldots, \frac{k}{2}+1, \frac{k}{2}, \frac{k}{2}, \frac{k}{2}-1, \ldots, 2, 1$$

when k is even, and

$$k, k-1, \ldots, \frac{k+1}{2}+1, \frac{k+1}{2}, \frac{k+1}{2}, \frac{k+1}{2}-1, \ldots, 2, 1$$

when k is odd. In either of the cases, $|\{\deg(u) : u \in V(G_k)\}| = k$. It now readily follows (having in mind that $\mathrm{diam}(G_k) = 2$) that $C_{\xi^{ce}}(G_k) = k$. This settles the theorem for diameter $d = 2$.

Let now $d = 2 + d'$, where $d' > 0$. Set $H_k = G_k \,\square\, Q_{d'}$. Distance Formula [15, Corollary 5.2] combined with Lemma 2.1 immediately implies that $\mathrm{diam}(H_k) = \mathrm{diam}(G_k) + \mathrm{diam}(Q_{d'}) = 2 + d' = d$. If (u, v) is an arbitrary vertex of H_k, then applying Distance Formula again and recalling that also the degree is an additive function in Cartesian product graphs, we get

$$\frac{\deg_{H_k}(u,v)}{\mathrm{ecc}_{H_k}(u,v)} = \frac{\deg_{G_k}(u) + \deg_{Q_{d'}}(v)}{\mathrm{ecc}_{G_k}(u) + \mathrm{ecc}_{Q_{d'}}(v)} = \frac{\deg_{G_k}(u) + d'}{\mathrm{ecc}_{G_k}(u) + d'}\,.$$

As the latter expression is independent of v, we infer that $C_{\xi^{ce}}(H_k) = C_{\xi^{ce}}(G_k) = k$. Hence H_k is a graph of diameter d with ξ^{ce}-complexity k as required. ■

3 On graphs with ξ^{ce}-complexity equal 1

In this section we consider the graphs G with $C_{\xi^{ce}}(G) = 1$ and demonstrate that their variety is quite large. The primarily reason why these graphs are interesting is the following.

Proposition 3.1 *If $C_{\xi^{ce}}(G) = 1$, then $\xi^{ce}(G) = |V(G)| \deg(v)/\mathrm{ecc}(v)$, where v is an arbitrary vertex of G. The conclusion in particular holds for any vertex-transitive graph.*

Proof. The first assertion follows immediately from (2). The second fact follows because graph automorphisms preserve degrees and distances. ■

In the rest of the section we search for graph G that are not vertex-transitive yet $C_{\xi^{ce}}(G) = 1$ holds. First we observe the following general properties on regular graphs.

Proposition 3.2 *Let G be a regular graph of order at least 3. Then*

(i) $C_{\xi^{ce}}(G) = 1$ *if and only if* $\mathrm{diam}(G) = \mathrm{rad}(G)$.

(ii) If $C_{\xi^{ce}}(G) = 1$, *then G is 2-connected.*

Proof. (i) If $\mathrm{rad}(G) \le t \le \mathrm{diam}(G)$, then there exists a vertex x of G with $\mathrm{ecc}(x) = t$ [2]. Since G is regular, it follows that $C_{\xi^{ce}}(G) = \mathrm{diam}(G) - \mathrm{rad}(G) + 1$ and the assertion follows.

(ii) Suppose on the contrary that G contains a cut-vertex v. Let w be a vertex of G such that $d(v, w) = \mathrm{ecc}(v)$. Let G_1 be the component of $G - v$ that contains w and let x be any neighbor of v that does not lie in G_1. (Such a neighbor exists since v is a cut-vertex.) Then $\mathrm{ecc}(x) > \mathrm{ecc}(v)$ and since G is regular, $C_{\xi^{ce}}(G) \ge 2$. ■

As a counterpart to Proposition 3.2(ii) consider the graph G from Fig. 3 which is not 2-connected yet $C_{\xi^{ce}}(G) = 1$. Note that $\deg(v)/\mathrm{ecc}(v) = 1$ holds for any vertex v of G.

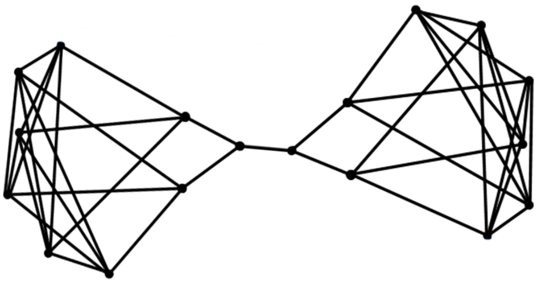

Figure 1: A graph G with $C_{\xi^{ce}}(G) = 1$

For a sporadic but interesting example consider the Gray graph, let us denote it here with Γ. The Gray graph is a cubic graph that is not vertex-transitive (but edge-transitive) [3]. Moreover, as it can be verified by hand or computer, $\mathrm{diam}(\Gamma) = \mathrm{rad}(\Gamma) = 6$. (For additional properties of the Gray graph and its drawings we refer to [20].) Hence Proposition 3.2(i) implies that $C_{\xi^{ce}}(\Gamma) = 1$. Using this example we can state:

Proposition 3.3 *There exists an infinite family of graphs G_k, $k \ge 0$, such that G_k is not vertex-transitive and* $C_{\xi^{ce}}(G) = 1$.

Proof. By the above we can set $G_0 = \Gamma$. For $k \ge 1$ let $G_k = \Gamma \,\Box\, Q_k$. Then

- $\mathrm{diam}(G_k) = \mathrm{diam}(\Gamma) + \mathrm{diam}(Q_k) = 6 + k$,

- $\mathrm{rad}(G_k) = \mathrm{rad}(\Gamma) + \mathrm{rad}(Q_k) = 6 + k$, and
- G_k is $(3 + k)$-regular graph.

Hence using Proposition 3.2(i) again we get that $C_{\xi^{\mathrm{ce}}}(G_k) = 1$. Finally, since $G \square H$ is vertex-transitive if and only if G and H are vertex-transitive [15, Theorem 6.17], and since $\mathcal{G}$ is not-vertex-transitive, G_k is not vertex-transitive. ■

Proposition 3.2(i) offers additional possibilities to construct graphs G that are not vertex-transitive and have $C_{\xi^{\mathrm{ce}}}(G) = 1$. Here is another construction. Let $d \geq 3$ and let G_d be the join of $C = C_k$ and Q_d, where $k = 2^d - d + 2$. (Recall that the join of (disjoint) graphs G and H is obtained from the disjoint union of G and H by adding all edges uv, where $u \in V(G)$ and $v \in V(H)$.) Then G_d is a $(2^d + 2)$-regular graph with $\mathrm{diam}(G_d) = \mathrm{rad}(G_d) = 2$. Hence $C_{\xi^{\mathrm{ce}}}(G_d) = 1$ by Proposition 3.2(i). That G_d is not vertex-transitive follows from the fact that a vertex of G_d that lies in Q_d does not lie in an induced cycle of length $k = 2^d - d + 2$. Indeed, an induced cycle of length k of G_d is either the cycle C or lies completely in Q_d, but an induced cycle of Q_d is of length at most 2^{d-1}. For the latter fact, actually for a stronger upper bound on the length of an induced cycle of a hypercube, see [6].

It seems interesting to consider graphs with the ξ^{ce}-complexity as large as possible. Since clearly $C_{\xi^{\mathrm{ce}}}(G) \leq |V(G)|$ holds, the extremal graphs are those for which $C_{\xi^{\mathrm{ce}}}(G) = |V(G)|$ holds. In a tree every diametrical vertex is of degree 1, hence there are no such graphs among trees. On the other hand, Fig. 2 displays an example of a graph G with $C_{\xi^{\mathrm{ce}}}(G) = |V(G)| = 7$.

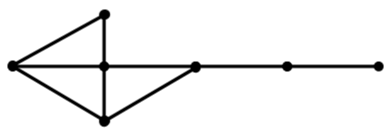

Figure 2: A graph with its ξ^{ce}-complexity equal to its order

It would be interesting to construct infinite families of graphs $\{G_n\}_{n\to\infty}$ such that $C_{\xi^{\mathrm{ce}}}(G_n) = |V(G_n)| = n$.

4 A cut method for eccentricity

The eccentricity of a vertex is the key ingredient for all our above developments. Hence we are justified to conclude the paper with the following result that can be understood as an instance of the cut method, cf. the recent survey [17] as well as an earlier one [16] on the cut method. More precisely, the next result is an instance of a *standard* cut method which means that it applies to partial cubes.

If uv is an edge of a graph G then set $W_{uv} = \{x : \ d_G(u,x) < d_G(v,x)\}$. W_{vu} is defined analogously. Now all is ready for the following result.

Theorem 4.1 *Let u be a vertex of a partial cube G. Then*

$$\mathrm{ecc}_G(u) = 1 + \max\{\mathrm{ecc}_{W_{vu}}(v) : \ uv \in E(G)\}\,.$$

Proof. Let u be a vertex of G and let w be a vertex such that $d_G(u,w) = \mathrm{ecc}_G(u)$. Let $P = uv\ldots w$ be a shortest u,w-path. Clearly, $v \in W_{vu}$ and, moreover, $v \in W_{vu}$ as well. Therefore $\mathrm{ecc}_{W_{vu}}(v) \geq d_{W_{vu}}(v,w)$. Since W_{vu} is an isometric (in fact, even convex) subgraph, $d_G(v,w) = d_{W_{vu}}(v,w)$ and so $\mathrm{ecc}_{W_{vu}}(v) \geq d_G(v,w)$. Since $d_G(u,w) = 1 + d_G(v,w)$ it follows that $\mathrm{ecc}_{W_{vu}}(v) \geq d_G(u,w) - 1 = \mathrm{ecc}_G(u) - 1$. In other words, $\mathrm{ecc}_G(u) \leq \mathrm{ecc}_{W_{vu}}(v) + 1$ which in turn implies that

$$\mathrm{ecc}_G(u) \leq 1 + \max\{\mathrm{ecc}_{W_{vu}}(v) : \ uv \in E(G)\}\,.$$

On the other hand, let x be a neighbor of u such that $\mathrm{ecc}_{W_{xu}}(x) = \max\{\mathrm{ecc}_{W_{vu}}(v) : uv \in E(G)\}$. Let x' be a vertex of W_{xu} such that $d_{W_{xu}}(x,x') = \mathrm{ecc}_{W_{xu}}(x)$. Since W_{xu} is isometric, we have $d_G(u,x') = 1 + d_{W_{xu}}(x,x') = 1 + \mathrm{ecc}_{W_{xu}}(x)$ and hence

$$\mathrm{ecc}_G(u) \geq 1 + \max\{\mathrm{ecc}_{W_{vu}}(v) : \ uv \in E(G)\}\,.$$

Combining the two inequalities the result follows. ■

Another point of view of Theorem 4.1 is that its equation is of dynamic programming nature. Indeed, the problem of computing the eccentricity of a given vertex in G is reduced to the smaller problems of computing the eccentricity in the induced subgraphs W_{vu}.

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