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SOME COMMENTS ON CO GRAPHS AND CI INDEX

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Abstract

In [13] co graphs are introduced and a formula is given for the PI index of these graphs. Based on this formula a new topological CI index is proposed. In this note it is observed that co graphs are precisely isometric subgraphs of hypercubes alias partial cubes. Some fact about partial cubes and their uses in chemical graph theory are listed. A couple of comments on the CI index are also given.

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1 Introduction

PI index is a topological index introduced in [14] that has received considerable attention in the last several years. In particular, its applications to QSRP/QSAR were studied and compared with the Wiener and the Szeged index [15, 16]. The PI index has similar discriminating power as the compared indices and in several cases it gives better result. Moreover, PI index is in principle easier to compute than the Wiener and the Szeged index.

The PI index has been computed for many classes of important molecular graphs, see [1, 2, 5, 6, 7, 17]. Very recently, John, Vizitiu, Cigher and Diudea obtained a formula for the computation of the PI index for the so-called co-graphs. In addition, motivated by the formula a new topological CI index was proposed and computed for armchair tubes, tori H$[q, 2p]$ and V$[q, 2p]$, and zig-zag tubes.

As it turns out, the co-graphs are precisely partial cubes, a class of graphs well-known and extensively studied in metric graph theory. These graphs were successfully applied in many areas of mathematics and elsewhere and were (independently) rediscovered several times. Since the paper [13] is another such case it seems appropriate to bring some fundamental facts about partial cubes to chemical graph theory. We do this in the subsequent section where it is in particular clarified that co-graphs are partial cubes. In the last section we give some comments on the CI index are suggest a possible extension of this index to non-bipartite graphs.

2 Co-graphs as partial cubes

Let us restate the definition of the co-graphs from [13]. Edges $e = uv$ and $f = xy$ of a bipartite graph are defined to be *codistant*, e co$f$, if for some k, $d(u, x) = d(v, y) = k$ and $d(u, y) = d(v, x) = k + 1$ or vice. The relation co is reflexive and transitive yet need not be transitive. The latter is demonstrate in [13] with a graph on 10 vertices. Note that a smaller example demonstrating this fact is provided with the complete bipartite graph $K_{2,3}$. Now, a bipartite graph G is a *co-graph* if the relation co is transitive (equivalently, if co is an equivalence relation).

Let us now turn to *partial cubes*—isometric subgraphs of hypercubes. (A graph H is an *isometric subgraph* of a graph G if $d_H(u,v) = d_G(u,v)$ for any vertices $u, v \in H$). The *Djoković-Winkler relation* Θ is defined on the edge set of a graph G in the following way. Let $uv, xy \in E(G)$, then $uv\Theta xy$ if

$$d(u,x) + d(v,y) \neq d(u,y) + d(v,x)\,.$$

In 1984 Winkler proved the following beautiful result [22]:

Theorem 2.1 *A connected graph is a partial cube if and only if it is bipartite and the relation Θ is transitive.*

Hence in a partial cube G the relation Θ partitions the edge set of G into equivalence classes that are called the Θ-*classes* of G.

It is clear that if two edges are in relation co then they are in relation Θ. On the other hand, the following observation is straightforward, see, for instance, [12, Lemma 2.3]:

Lemma 2.2 *Let G be a bipartite graph and $uv\Theta xy$. Then the notation can be chosen such that $d(u,x) = d(v,y) = d(u,y) - 1 = d(v,x) - 1$.*

Putting the above considerations together we have the following key observation:

Proposition 2.3 *A graph G is a co-graph if and only if G is a partial cube.*

We conclude the section by some relevant remarks about partial cubes.

- This is not the first time that partial cubes are applied in chemical graph theory. Probably the first such application goes back to [20] where it was observed that any benzenoid graph belongs to the class of partial cubes and consequently, the Wiener index of a benzenoid graph can be computed by a simple approach.

- The observation that benzenoid graphs are partial cubes let to the so-called "cut-method" that gave several successfully applications, see [3, 8, 9, 11, 21].

- The graph of an arbitrary phenylene (a chemical compounds in which the carbon atoms form 6- and 4-membered cycles) is also a partial cube [19, 10].

3 On the CI index

Let G be a partial cube and $E_1, \ldots, E_k$ its Θ-classes. Then the PI index of G, $PI(G)$, can be expressed as

$$PI(G) \;=\; \|G\|^2 - \sum_{i=1}^{k} |E_i|^2 \,, \tag{1}$$

where $\|G\|$ denoted the number of edges of G [13]. We note that (1) is a special case of the formula that gives the PI index for any graph that admits the so-called PI-partition, see [18] for details.

Suppose G is a plane bipartite graph with isometric faces. An edge f of a face F is in relation Θ to its antipodal edge f' on F. Then a *quasi-orthogonal cut* with respect to a given edge is the smallest subset of edges closed under this operation. (Note that in a partial cube, quasi-orthogonal cuts are precisely the Θ-classes of G.) Motivated by formula (1), the CI index was introduced in [13] for plane bipartite graphs with isometric faces using the same formula, expect that the edge sets $E_1, \ldots, E_k$ are now quasi-orthogonal cuts.

Note that $CI(G) = 0$ provided that G contains a single quasi-orthogonal cut. A sporadic example of such a graph is shown in Fig. 1.

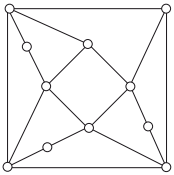

Figure 1: Graph G with $CI(G) = 0$

An infinite series of such examples is provided by complete bipartite graphs $K_{2,2k+1}$, $k \geq 1$, that is, $CI(K_{2,2k+1}) = 0$ for any $k \geq 1$. On the other hand, $CI(K_{2,2k}) = (4k)^2 - 2 \cdot (2k)^2 = 8k^2$. This shows that similar graphs can have arbitrarily different CI indices. Of course, the complete bipartite graphs $K_{2,n}$ are not chemical graphs and it could be that such situations do not happen (or are rare) for chemical graphs. The examples computed in [13] indicate that this might indeed be the case. In any case, possible applications of the CI index to QSRP/QSAR still need to be explored.

Finally, it would certainly be desirable to expend the CI index to (plane) graphs that are not bipartite. In this respect the approach from [4] using the so-called alternating cuts seems to be a natural option.

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