JOURNAL OF MATHEMATICAL NANOSCIENCE

JMNS

Vol. 4, No. 1, 2014, 37-44

On the Zagreb indices of overfull molecular graphs

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ABSTRACT. Let G be a connected graph on n vertices. An overfull graph is a graph whose number of its edges is greater than $\Delta \times [n/2]$, where Δ is the maximum degree of vertices in G. In this paper, we compute the Zagreb indices of overfull molecular graphs.

Keywords: overfull graph, Zagreb indices, molecular graph.

1. INTRODUCTION

Thought this paper all graphs are connected simple graphs. Let G be a graph with n vertices and m edges, then G is overfull graph if $m > \Delta(G)[n/2]$. It is easy to see that the number of vertices of an overfull graph is an odd number.

The k - edge coloring of a graph is an assignment of k colors to the edges of the graph so that adjacent edges have different colors. The minimum required number of colors for the edges of a given graph is called the edge chromatic number of the graph and it is denoted by $\chi'(G)$.

Here, in the next section, we determine n-th extremal overfull graphs where $n \leq 10$. Throughout this paper, our notation is standard and mainly taken from [1,6].

2. Results and Discussion

In this section we compute some bounds for overfull graphs and then we determine the Zagreb indices of overfull molecular graphs. To do this, we need to recall some definitions.

Let $\Delta(G)$ be the maximum degree of vertices of graph G. Obviously, $\chi'(G) \geq \Delta(G)$ and by Vizing's theorem $\chi'(G) = \Delta(G)+1$. In other words, $\chi'(G) = \Delta(G)$ or $\chi'(G) = \Delta(G)+1$. The graph G is said to be of class 1 whenever, $\chi'(G) = \Delta(G)$ and otherwise, it is said to be of class 2.

The concept of overfull graph has improved our understanding of the edge chromatic properties of graphs. Chetwynd and Hilton [2] have formulated the following conjecture, according to which the reason for a vaste category of graphs to be class 2 is that they contain an overfull subgraph with the same maximum degree:

Conjecture. A graph G with $\Delta(G) > |V(G)|/3$ is class 2 if and only if it contains an overfull subgraph H such that $\Delta(G) = \Delta(H)$.

It should be noted that, this conjecture is solved only under special conditions. For more details one can see the Refs [5].

Let f be an arbitrary edge of the cycle C_n on n vertices. Connect $(n\text{-}3)/2$ new independent edges to C_n parallel with f and then join an endpoint of f to the remained vertex of degree 2, the resulted graph is an overfull graph and we denote it by $C_n + \frac{n\text{-}1}{2}e$, see Figure 1.

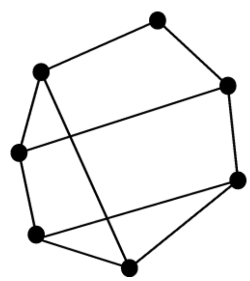

Figure 1. The graph $C_7 + 3e$.

In continuing, by $K_n - me$ we mean that m independent edges removed from K_n. In [3] Ghorbani, computed the n-th maximal and minimal overfull graphs for $n \leq 4$. In other words, he proved the following theorem:

Theorem 1.

i) Let $n \geq 3$, among all n-vertex overfull graphs, the complete graph K_n is maximal and the cycle C_n is minimal.

ii) Let $n \geq 5$, then the second maximal overfull graph on n vertices is K_n - e, and the second minimal is $C_n + \frac{n\text{-}1}{2}e$.

iii) Let $n \geq 7$ then the third maximal overfull graph on n vertices is K_n - $2e$, and the third minimal can be constructed by removing an edge from a 4-regular graph, see Figure 2.

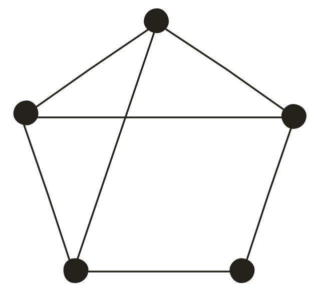

Figure 2. The third maximal overfull graph for $n = 5$.

iv) For $n \geq 9$ the fourth maximal overfull graph is isomorphic with K_n - $3e$ and the fourth minimal is a 4-regular graph. For $n = 5$, the cycle graph C_5 is the fourth maximal overfull graph and for $n = 7$ the graph $G+ 3e$ is the fourth maximal overfull graph, where G is a 4-regular graph.

Theorem 2[3]. Trees and unicycle graphs are not overfull. Moreover, a graph with a pendant vertex is not overfull.

Here, by continuing the methods of [3], we compute the n-th extremal overfull graph, where $n \leq 10$. Let G be a connected graph on n vertices, $n \geq 7$. One can see easily that for $n = 7$ the graph $G + 2e$ is the fifth maximal overfull graph, where G is a 4-regular graph. On the other hand, we have the following theorem:

Theorem 3. Let $n \geq 9$ then the fifth maximal overfull graph on $n = 9$ vertices is $G + 4e$, where G is a 6-regular graph, the fifth maximal overfull graph on $n > 9$ is $K_n - 4e$ and the fifth minimal is $H + \frac{n\text{-}3}{2}e$, where H is a 4-regular graph.

Theorem 4. Let $n \geq 7$ then

- If $n = 7$ then the sixth maximal overfull graph is a 4-regular graph,
- If $n = 9$ then the sixth maximal overfull graph is $G + 3e$ where G is a 6-regular graph,
- If $n = 11$ then the sixth maximal overfull graph is $G + 5e$ where G is a 8-regular graph,
- If $n \geq 13$ then the sixth maximal overfull graph is $K_n - 5e$,
- The sixth minimal is $H + \frac{n\text{-}3}{2}e$, where H is a 4-regular graph.

Proof. First we compute the sixth extremal graph. It is obvious that by removing an edge from fifth maximal overfull graph, the resulted graph is not overfull. So, the sixth maximal overfull graph constructed from the fifth maximal by removing an edge from the $\Delta(G)$-vertex. It follows that the sixth maximal is a 4-regular graph. For $n = 9$, by

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removing an edge from fifth maximal overfull graph, the sixth maximal is $G + 3e$. For n = 11, we cannot remove an edge from the fifth maximal, because the resulted graph is not overfull. Thus, by removing two independent edges from $\Delta(G)$-vertex, the sixth maximal is an 8-regular graph isomorphic with $G + 5e$. Finally for $n \geq 13$, the sixth minimal can be obtained by adding a new edge to the fifth minimal. It is clear that the sixth minimal is isomorphic with $H+\frac{n\text{-}1}{2}e$ where H is a 4-regular graph.

Theorem 5. Let $n \geq 7$ then

- If n =7 then the seventh maximal overfull graph is a graph $G-e$, where G is a 4-regular graph,
- If n = 9 then the seventh maximal overfull graph is $G + 2e$, where G is a 6-regular graph,
- If n = 11 then the seventh maximal overfull graph is $G + 4e$, where G is a 8-regular graph,
- If n = 13 then the seventh maximal overfull graph is $G + 6e$, where G is a 10-regular graph,
- If $n \geq 15$ then the seventh maximal overfull graph is $K_n - 6e$,
- The seventh minimal is $H - 2e$, where H is a 6-regular graph.

Proof. The proof of all maximal cases is similar to the proof of the last theorem. For the seventh minimal, it should be noted that by adding a new edge, the resulted graph is not overfull. Let the seventh, minimal can be constructed by adding x independent edges where $x > 1$. Hence, we have

$$2n+\frac{n-1}{2}+x>6\frac{n-1}{2}\Rightarrow\frac{5n-1}{2}+x>\frac{6n-6}{2}.$$

Therefore,

$$x>\frac{6n-6}{2}-\frac{5n-1}{2}=\frac{n-5}{2}.$$

This implies that by adding at least $(n$-3)/2 new independent edges to the sixth minimal, we achieve the seventh minimal. In other words, the seventh minimal is H-2e in which H is a 6-regular graph.

Theorem 6. Let $n \geq 7$ then

- If n =7 then the eighth maximal overfull graph is a graph $C_7 + 3e$,
- If n = 9 then the eighth maximal overfull graph is a 6-regular graph,
- If n = 11 then the eighth maximal overfull graph is $G + 3e$, where G is a 8-regular graph,
- If n = 13 then the eighth maximal overfull graph is $G + 5e$, where G is a 10-regular graph,
- If n = 15 then the eighth maximal overfull graph is $G + 7e$, where G is a 12-regular graph,
- If $n \geq 17$ then the eighth maximal overfull graph is $K_n - 7e$,
- The eighth minimal is H - e, where H is a 6-regular graph.

Proof. Use Theorems 4,5.

By continuing our method, we can construct the ninth and tenth extremal overfull graphs. Because of similarity, we express the Theorems 7,8 without proof.

Theorem 7. Let $n \geq 7$ then

- If n =7 then the ninth maximal overfull graph is C_7,
- If n = 9 then the eighth maximal overfull graph is a graph G-e, where G is a 6-regular graph,
- If n = 11 then the ninth maximal overfull graph is G + 2e, where G is a 8-regular graph,
- If n = 13 then the ninth maximal overfull graph is G + 4e, where G is a 10-regular graph,
- If n = 15 then the ninth maximal overfull graph is G + 6e, where G is a 12-regular graph,
- If n = 17 then the ninth maximal overfull graph is G + 8e, where G is a 14-regular graph,
- If $n \geq 19$ then the ninth maximal overfull graph is $K_n - 8e$,
- The ninth minimal is a 6-regular graph.

Theorem 8. Let $n \geq 9$ then

- If n = 9 then the tenth maximal overfull graph is a graph G - 2e, where G is a 6-regular graph,
- If n = 11 then the tenth maximal overfull graph is G, where G is a 8-regular graph,
- If n = 13 then the tenth maximal overfull graph is G + 3e, where G is a 10-regular graph,
- If n = 15 then the tenth maximal overfull graph is G + 5e, where G is a 12-regular graph,
- If n = 17 then the tenth maximal overfull graph is G + 7e, where G is a 14-regular graph,
- If n = 19 then the tenth maximal overfull graph is G + 9e, where G is a 16-regular graph,
- If $n \geq 21$ then the tenth maximal overfull graph is $K_n - 9e$,
- The tenth minimal is $H + \frac{n-5}{2}e$, where H is a 6-regular graph.

3. Computing the Zagreb indices of overfull molecular graphs

Let G be an overfull graph with maximum degree Δ. First, we classify all such graphs up to isomorphism, for $1 \leq \Delta \leq 4$. In Theorems 9 – 11, we construct these graphs. In the following Theorems, let G is an overfull graph. It should be noted that, according to Theorem 2 such graphs have no pendant ices Hence, if $\Delta = 1$, then G is not overfull.

Theorem 9. Let $\Delta = 2$, then $G \cong C_n$.

Proof. According to [3, Lemma 5] the proof is clear.

Theorem 10. Let $\Delta = 3$, then $G \cong C_n + \frac{n-1}{2}e$ $(n \geq 4)$.

Proof. Let G be an overfull graph with $\Delta = 3$. Let n_i be the number of vertices of degree i (i = 1, 2, 3, ...) in graph G. Since an overfull graph has no pendant vertex, we have

$$\begin{cases} n_2 + n_3 = n \\ 2n_2 + 3n_3 = 2m \end{cases}. \tag{1}$$

Since G is overfull, then $2m > 3(n\text{-}1)$ and by Eq. (1) we have $n_2 \leq 2$. This implies that $n_2 = 1$ or 2. If $n_2 = 1$, then clearly $G \cong C_n + \frac{n-1}{2}e$ and if $n_2 = 2$, then $2n_2 + 3n_3$ is an odd number, a contradiction with Eq. (1).

Theorem 11. Let $\Delta = 4$, then G is isomorphic with one of the following graphs:

- A 4-regular graph,
- A graph constructed from a 4-regular graph with n-1 vertices by adding a new vertex to middle of an arbitrary edge,
- A graph with two vertices of degree 3 and the others are of degree 4.

Proof. Similar to the proof of Theorem 10, we have

$$\begin{cases} n_2 + n_3 + n_4 = n \\ 2n_2 + 3n_3 + 4n_4 = 2m \end{cases}. \tag{2}$$

Since G is overfull, then $2m > 4(n\text{-}1)$ and by Eq. (2) we have $2n_2 + n_3 \leq 3$. Thus by solving these equations, we find that the following cases are impossible:

- $n_2 = 0$, $n_3 = 1$,
- $n_2 = 0$, $n_3 = 3$,
- $n_2 = n_3 = 1$,

This yields the following cases:

- $n_2 = n_3 = 0$, in this case it is clear that G is 4-regular and so the first claim is proved.
- $n_2 = 1$ and $n_3 = 0$, thus Eq.(2) yields a vertex of degree 2 and (n-1) vertices of degree 4. According to the second Eq.(2) we have exactly $2m = 4(n\text{-}1) + 2$ edges and this completes the proof of second claim.
- $n_2 = 0$ and $n_3 = 2$, by substituting these values in Eq.(2) the proof is completed.

Corollary 12. There is no a cubic overfull molecular graph.

Proof. Let G be a cubic molecular graph on n vertices. If n is even, then G is not overfull. If n is odd, then we get a contradiction, since the sum of degrees of vertices in a graph is an even number.

Let Σ be the class of finite graphs. A ***topological index*** is a function $\mu : \Sigma \to R^{+}$ with this property that $\mu(G) = \mu(H)$ if G and H are isomorphic. Obviously, the number of vertices and the number of edges are topological index.

The ***Zagreb indices*** have been introduced in 1972 by Gutman and Trinajstić [4]. They are defined as:

$$M_1(G) = \sum_{v\in V(G)} (d(v))^2 \text{ and } M_2(G) = \sum_{uv\in E(G)} d(u)d(v),$$

where degree of vertex u is denoted by $d(u)$.

Theorem 13. Let G be a overfull molecular graph. Then the Zagreb indices of G are one of the following pairs:

$$(4n,4n),(9n\text{-}5,(27n\text{-}11)/2),(12n,24n),(16n+4,32n),(32n\text{-}14,32n\text{-}40).$$

Proof. Let G be a overfull molecular graph, the following cases hold:

1) if $\Delta = 2$, then $M_1(G) = M_2(G) = 4n$.
2) if $\Delta = 3$, then clearly one vertex is of degree two and the others are of degree three. Further, G has $n + (n\text{-}1)/2$ edges. This means that

$$M_1(G) = 2\times(2+3) + \frac{3n-5}{2}(3+3) = 9n-5,$$
$$M_2(G) = 2\times(2\times3) + \frac{3n-5}{2}(3\times3) = \frac{27n-11}{2}.$$

3) if $\Delta = 4$, then the following subcases hold:

- graph G is 4-regular and so

$$M_1(G) = m(4+4) = 12n,\ M_2(G) = m(4\times4) = 24n.$$

  Since G has n-1 vertices of degree four and one vertex of degree two, it has $2n$+1 edges and thus

$$M_1(G) = 2\times(2+4) + (2n-1)(4+4) = 16n+4,$$
$$M_2(G) = 2\times(2\times4) + (2n-1)(4\times4) = 32n.$$

- graph G has two vertices of degree three and the others are of degree four. Therefore, G has $2n$-1 edges and so

$$M_1(G) = 6\times(3+4) + (2n-7)(4+4) = 32n-14,$$
$$M_2(G) = 6\times(3\times4) + (2n-7)(4\times4) = 32n-40.$$

This completes the proof.

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