第49卷第3期 中国科学技术大学学报 Vol. 49, No. 3
2019年3月 JOURNAL OF UNIVERSITY OF SCIENCE AND TECHNOLOGY OF CHINA Mar. 2019

文章编号:0253-2778(2019)03-0195-04

Maximum augmented Zagreb index of graphs with given vertex bipartiteness

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Abstract: Augmented Zagreb index (AZI) of a graph is widely used to study the heat information of heptanes and octanes in chemistry. Here graphs with given vertex bipartiteness were studied. The extremal graph having maximum AZI was given. The relationship between the extremal graph and complete bipartite graph was analyzed.

Key words: augmented Zagreb index; complete bipartite graph; vertex bipartiteness

CLC number: O157.5 **Document code**: A doi:10.3969/j.issn.0253-2778.2019.03.003

2010 Mathematics Subject Classification: 05C40

Citation: GAO Fang, ZHA Shuping, WANG Zhen, et al. Maximum augmented Zagreb index of graphs with given vertex bipartiteness[J]. Journal of University of Science and Technology of China, 2019,49(3): 195-198.
高芳,查淑萍,王贞,等. 给定点二部度的图的极大增强 Zagreb 指数[J]. 中国科学技术大学学报, 2019,49(3):195-198.

给定点二部度的图的极大增强 Zagreb 指数

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摘要:图的增强 Zagreb 指数在化学中被广泛地用于研究庚烷和辛烷的热量信息. 研究给定点二部度的图,得到了达到极大增强 Zagreb 指数的极图,并分析了这类极图与完全二部图的关系.

关键词:增强 Zagreb 指数;完全二部图;点二部度

0 Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. A graph G is called a bipartite graph when its vertex set can be partitioned into two disjoint parts V_1, V_2 such that all edges of G meet both V_1 and V_2[1]. The subgraph of G induced by V', denoted by $\langle V' \rangle$, is the subgraph $G'=(V'(G'), E'(G'))$ of G in which G' has the vertex set V', and for all $u, v \in V'$, $e=$

Received: 2017-05-02; **Revised**: 2018-01-21

Foundation item: Supported by Talent Introduction Project of Anhui Science and Technology University (XWYJ201801), the Research Project of Chizhou University (2015ZR005; 2016ZR008; 2016XJXTD02; 2017ZRZ009), the Project of the Outstanding Young Talent Support Program of the Universities of Anhui Province (gxyq2019107).

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$uv \in E(G)$ if and only if $e \in E'(G')$. The vertex bipartiteness of a graph G, denoted by $v_b(G)$, is the minimum number of vertices whose deletion from G results in a bipartite graph[2]. Robbiano et al.[3] researched the maximum spectral radius and maximum signless Laplacian spectral radius with a bounded vertex bipartiteness number. Liu and Pan[4] characterized the graphs which have the minimum Kirchhoff index with a vertex bipartiteness number.

The augmented Zagreb index (AZI) of graphs was proposed by Furtula et al.[5]. It is denoted by AZI(G) and defined as

$$\mathrm{AZI}(G)=\sum_{uv\in E(G)}\left(\frac{d_u d_v}{d_u+d_v-2}\right)^3,$$

where d_u and d_v are the degree of the vertex u and v in G, respectively. The AZI is a valuable index to calculate the heat information of heptanes and octanes in chemistry. In recent years, researchers have obtained an increasing number of results on AZI. Huang et al.[6-7] have given the upper and lower bound on AZI, and ordered the AZI of connected graphs. Sun et al.[8] have researched the AZI of line, subdivision and total graphs.

In this paper, we analyze the maximum AZI among graphs with a given vertex bipartiteness number $v_b(G)$. When the vertices number n and the bipartiteness number m are given, the maximum AZI on vertex bipartiteness graphs is solved. The extremal graph is related with the complete bipartite graph and complete graph.

1 Maximum AZI of the complete bipartite graph

The complete graph K_n is a graph with n vertices, and any two different vertices are connected by an edge. A complete bipartite graph K_{n_1,n_2} is a bipartite graph, with a bipartition $\{V_1, V_2\}$, where $|V_1|=n_1$, $|V_2|=n_2$, and arbitrarily two vertices $u\in V_1$ and $v\in V_2$ are connected by an edge. The complement graph $\overline{G}$ of graph G, is the graph with $V(\overline{G})=V(G)$, and $E(\overline{G})=\{uv: uv\notin E(G)\}$.

Let G_1 and G_2 be two vertex-disjoint graphs, the join of G_1 and G_2 is denoted by $G_1 \vee G_2$, such that $V(G_1\vee G_2)=V(G_1)\cup V(G_2)$, and

$$E(G_1\vee G_2)=E(G_1)\cup E(G_2)\cup \{uv: u\in V(G_1), v\in V(G_2)\}.$$

Thus K_{n_1,n_2} can be written as $\overline{K}_{n_1}\vee\overline{K}_{n_2}$.

Lemma 1.1[6] The AZI is monotonic increasing in the number of edges in a graph. Then for $e\notin E(G)$, AZI(G)<AZI($G+e$).

We in the following calculate the maximum AZI on K_{n_1,n_2}.

Theorem 1.1 Let K_{n_1,n_2} be a complete bipartite graph with n vertices, then the following result holds:

① If n is even, then

$$\mathrm{AZI}(K_{n_1,n_2})\leqslant\frac{n^8}{256(n-2)^3}.$$

② If n is odd, then

$$\mathrm{AZI}(K_{n_1,n_2})\leqslant\frac{(n^2-1)^4}{256(n-2)^3}.$$

Proof Note that

$$\mathrm{AZI}(K_{n_1,n_2})=\sum_{uv\in K_{n_1,n_2}}\left(\frac{d_u d_v}{d_u+d_v-2}\right)^3=n_1n_2\left(\frac{n_1n_2}{n_1+n_2-2}\right)^3=\frac{(n_1n_2)^4}{(n_1+n_2-2)^3},$$

$$\mathrm{AZI}(K_{n_1-1,n_2+1})=\frac{(n_1-1)^4(n_2+1)^4}{(n_1+n_2-2)^3}=\frac{[(n_1-1)(n_2+1)]^4}{(n_1+n_2-2)^3}.$$

If $n_1-1\geqslant n_2+1$, then

$$n_1n_2<(n_1-1)(n_2+1),$$
$$\mathrm{AZI}(K_{n_1-1,n_2+1})>\mathrm{AZI}(K_{n_1,n_2}).$$

Then we have that if n is even, then

$$\mathrm{AZI}(K_{n_1,n_2})\leqslant K_{\frac{n}{2},\frac{n}{2}}=\frac{n^8}{256(n-2)^3};$$

and that if n is odd, then

$$\mathrm{AZI}(K_{n_1,n_2})\leqslant K_{\frac{n-1}{2},\frac{n+1}{2}}=\frac{(n^2-1)^4}{256(n-2)^3}.$$

2 Maximum AZI of vertex bipartiteness graphs

Let $B_{n,m}$ be the set of graphs with n vertices, and the vertex bipartiteness $v_b(G)\leqslant m$, then

$B_{n,m}=$
$\{G=(V(G),E(G)):|V(G)|=n,v_b(G)\leqslant m\}$.

Theorem 2.1 Let $1\leqslant m\leqslant n-3$, $n\geqslant 3$, $G\in B_{n,m}$, then the following results hold:

① If $n-m$ is even, then $\mathrm{AZI}(\widetilde{G})\geqslant \mathrm{AZI}(G)$, where $\widetilde{G}=K_m\vee(\overline{K_{\frac{n-m}{2}}}\vee\overline{K_{\frac{n-m}{2}}})$. The equality holds if and only if $\widetilde{G}\cong G$, and

$$\mathrm{AZI}(\widetilde{G})=\frac{m(m-1)(n-1)^6}{16(n-2)^3}+\frac{m(n-m)(n-1)^3(n+m)^3}{8(3n+m-4)^3}+\frac{(n-m)^2(n+m)^6}{256(n+m-2)^3}.$$

② If $n-m$ is odd, then $\mathrm{AZI}(\widetilde{G})\geqslant \mathrm{AZI}(G)$, where $\widetilde{G}=K_m\vee(\overline{K_{\frac{n-m-1}{2}}}\vee\overline{K_{\frac{n-m+1}{2}}})$. The equality holds if and only if $\widetilde{G}\cong G$, and

$$\mathrm{AZI}(\widetilde{G})=\frac{m(m-1)(n-1)^6}{16(n-2)^3}+m(n-1)^3\left[\frac{(n+m+1)^3}{(3n+m-5)^3}+\frac{(n+m-1)^3}{(3n+m-7)^3}\right]+\frac{[(n-m)^2-1][(n+m)^2-1]^3}{256(n+m-2)^3}.$$

Proof For any $G\in B_{n,m}$, let $\widetilde{G}\in B_{n,m}$, such that $\mathrm{AZI}(\widetilde{G})\geqslant\mathrm{AZI}(G)$. Suppose that the vertex bipartiteness of graph $\widetilde{G}$ is m', and $i_1,i_2,\cdots,i_{m'}$ are the vertices in $V(\widetilde{G})$, such that $\widetilde{G}/\{i_1,i_2,\cdots,i_{m'}\}$ is a bipartite graph with a bipartition $\{V_1,V_2\}$, where $|V_1|=n_1$ and $|V_2|=n_2$, then $n=n_1+n_2+m'$.

Suppose that there exist $v_1\in V_1, v_2\in V_2$, and v_1,v_2 are not adjacent, let $\widetilde{G}^+=\widetilde{G}+uv$, obviously $\widetilde{G}^+\in B_{n,m}$. By Lemma 1.1, we have $\mathrm{AZI}(\widetilde{G}^+)\geqslant\mathrm{AZI}(\widetilde{G})$, which is a contradiction. Therefore any two vertices $v_1\in V_1, v_2\in V_2$ are adjacent, implying that $\widetilde{G}/\{i_1,i_2,\cdots,i_{m'}\}$ is a complete bipartite graph. Similarly, we obtain that $\langle\{i_1,i_2,\cdots,i_{m'}\}\rangle$ is a complete graph,

$$\widetilde{G}=K_{m'}\vee K_{n_1,n_2}=K_{m'}\vee(\overline{K_{n_1}}\vee\overline{K_{n_2}}).$$

Assume $m'<m$, then

$$n_1+n_2=n-m'>n-m\geqslant 3.$$

It implies that $n_1\geqslant 2$ or $n_2\geqslant 2$.

Suppose that $n_1\geqslant 2$, then

$$\widetilde{G}=K_{m'}\vee(\overline{K_{n_1}}\vee\overline{K_{n_2}})$$

has a subgraph $K_{m'+1}=K_{m'}\vee K_1$, which is a join of the graph $K_{m'}$ and a vertex of K_{n_1}. It is easy to check that

$$G'=K_{m'+1}\vee(\overline{K_{n_1-1}}\vee\overline{K_{n_2}})\in B_{n,m}.$$

By calculation, the edge number of $\widetilde{G}=K_{m'}\vee(\overline{K_{n_1}}\vee\overline{K_{n_2}})$ is $\frac{m'(m'-1)}{2}+m'n_1+m'n_2+n_1n_2$ and the edge number of

$$G'=K_{m'+1}\vee(\overline{K_{n_1-1}}\vee\overline{K_{n_2}})\in B_{n,m}$$

is $\frac{(m'+1)m'}{2}+(m'+1)(n_1-1)+(m'+1)n_2+(n_1-1)n_2$.

Then graph $\widetilde{G}$ has n_1-1 edges less than G', by Lemma 1.1, we have $\mathrm{AZI}(\widetilde{G})<\mathrm{AZI}(G')$, which is a contradiction, thus $m'=m$. Therefore we have

$$\widetilde{G}=K_m\vee(\overline{K_{n_1}}\vee\overline{K_{n_2}}).$$

The degree d_u of vertex u is

$$d_u=\begin{cases}n-1, & u\in K_m;\\ n-n_1, & u\in\overline{K_{n_1}};\\ n-n_2, & u\in\overline{K_{n_2}};\end{cases}$$

so the AZI of graph $\widetilde{G}$ is

$$\mathrm{AZI}(\widetilde{G})=\sum_{uv\in\widetilde{G}}\left(\frac{d_u\cdot d_v}{d_u+d_v-2}\right)^3=\sum_{u,v\in K_m}\left(\frac{d_ud_v}{d_u+d_v-2}\right)^3+\sum_{u\in K_m,v\in\overline{K_{n_1}}}\left(\frac{d_ud_v}{d_u+d_v-2}\right)^3+\sum_{u\in K_m,v\in\overline{K_{n_2}}}\left(\frac{d_ud_v}{d_u+d_v-2}\right)^3+\sum_{u\in\overline{K_{n_1}},v\in\overline{K_{n_2}}}\left(\frac{d_ud_v}{d_u+d_v-2}\right)^3=$$

$$\frac{m(m-1)}{2}\left[\frac{(n-1)(n-1)}{n-1+n-1-2}\right]^3+mn_1\left[\frac{(n-1)(n-n_1)}{2n-n_1-3}\right]^3+mn_2\left[\frac{(n-1)(n-n_2)}{2n-n_2-3}\right]^3+n_1n_2\left[\frac{(n-n_1)(n-n_2)}{2n-n_1-n_2-2}\right]^3.$$

Let $\widehat{G}=K_m \vee (\overline{K_{n_1-1}} \vee \overline{K_{n_2+1}})$, then

$$\mathrm{AZI}(\widehat{G})=\frac{m(m-1)}{2}\left[\frac{(n-1)(n-1)}{2n-4}\right]^3+ m(n_1-1)\left[\frac{(n-1)(n-n_1+1)}{2n-n_1-2}\right]^3+ m(n_2+1)\left[\frac{(n-1)(n-n_2-1)}{2n-n_2-4}\right]^3+ (n_1-1)(n_2+1)\left[\frac{(n-n_1+1)(n-n_2-1)}{2n-n_1-n_2-2}\right]^3,$$

$$\mathrm{AZI}(\widetilde{G})-\mathrm{AZI}(\widehat{G})=m(n-1)^3\left[\frac{n_1(n-n_1)^3}{(2n-n_1-3)^3}+\frac{n_2(n-n_2)^3}{(2n-n_2-3)^3}-\frac{(n_1-1)(n-n_1+1)^3}{(2n-n_1-2)^3}-\frac{(n_2+1)(n-n_2-1)^3}{(2n-n_2-4)^3}\right]+ \frac{1}{(2n-n_1-n_2-2)^3}\left[n_1n_2(n-n_1)^3(n-n_2)^3-(n_1-1)(n_2+1)(n-n_1+1)^3(n-n_2-1)^3\right].$$

If $n_1-1\geqslant n_2+1$, then $\mathrm{AZI}(\widetilde{G})<\mathrm{AZI}(\widehat{G})$. Therefore, if $n-m$ is even, then we have

$$n_1=n_2=\frac{n-m}{2}.$$

That is to say $\widetilde{G}=K_m \vee (\overline{K_{\frac{n-m}{2}}} \vee \overline{K_{\frac{n-m}{2}}})$, and

$$\mathrm{AZI}(\widetilde{G})=\frac{m(m-1)}{2}\left[\frac{(n-1)(n-1)}{n-1+n-1-2}\right]^3+ 2m\frac{n-m}{2}\left[\frac{(n-1)(n+m)/2}{n-1+(n+m)/2-2}\right]^3+ \frac{n-m}{2}\frac{n-m}{2}\left(\frac{(n+m)/2\cdot(n+m)/2}{(n+m)/2+(n+m)/2-2}\right)^3= \frac{m(m-1)(n-1)^6}{16(n-2)^3}+ \frac{m(n-m)(n-1)^3(n+m)^3}{8(3n+m-4)^3}+ \frac{(n-m)^2(n+m)^6}{256(n+m-2)^3}.$$

If $n-m$ is odd, then we have

$$n_1=\frac{n-m+1}{2},\ n_2=\frac{n-m-1}{2}.$$

That is to say $\widetilde{G}=K_m \vee (\overline{K_{\frac{n-m+1}{2}}} \vee \overline{K_{\frac{n-m-1}{2}}})$, and

$$\mathrm{AZI}(\widetilde{G})=\frac{m(m-1)}{2}\left[\frac{(n-1)(n-1)}{n-1+n-1-2}\right]^3+ m\frac{n-m-1}{2}\left[\frac{(n-1)(m+\frac{n-m+1}{2})}{n-1+m+\frac{n-m+1}{2}-2}\right]^3+ m\frac{n-m+1}{2}\left[\frac{(n-1)(m+\frac{n-m-1}{2})}{n-1+m+\frac{n-m-1}{2}-2}\right]^3+ \frac{n-m-1}{2}\frac{n-m+1}{2}\cdot\left[\frac{(m+\frac{n-m-1}{2})(m+\frac{n-m+1}{2})}{m+\frac{n-m-1}{2}+m+\frac{n-m+1}{2}-2}\right]^3=$$

$$\frac{m(m-1)(n-1)^6}{16(n-2)^3}+ m(n-1)^3\frac{(n+m-1)^3}{(3n+m-7)^3}+ m(n-1)^3\frac{(n+m+1)^3}{(3n+m-5)^3}+ \frac{[(n-m)^2-1][(n+m)^2-1]^3}{256(n+m-2)^3}.$$

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