

Minimum absolute deviation covering chromatic energy of graphs

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Abstract

The study of Minimum Absolute Deviation Covering Chromatic Energy explores the relationship between graph structures and energy metrics, providing insights into optimal colouring strategies. We are introducing minimum absolute deviation of a graph covering chromatic energy G corresponding to minimum covering C of some standard graphs and their bounds also established.

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1. Introduction

In the field of chemistry, the graph energy [1, 2] plays a crucial role in determining the total molecular π -electron energy, which is derived from graph energy, wherein each carbon atom is represented as a vertex and each carbon-carbon bond is represented as an edge. In this study, we computed the minimum absolute deviation encompassing the partition energy of graphs subject to specified bounds.

For a simple graph $G = (V, E)$, a covering set $C \subseteq V$ is such that every $e \in E$ is having at least one end vertex is from C , which is termed as ‘covering set’ of G . Minimum covering (MC) set is any covering set [2, 4] with least cardinality. Allocating colours to vertices of a graph G so that every pair of vertices should get different colours when they are adjacent is colouring of G . The least number of colours to colour G is called its ‘chromatic number’, $\chi(G)$. Let C be the MC set for a graph $G = (V, E)$ consisting of ‘ n ’ vertices. Then the MC chromatic (MCCh) matrix of a graph ‘ G ’ is of order $n \times n$ and is as follows:

$$A_{CCh}(G) = \begin{cases} -1; & \text{any two vertices which are non adjacent with same colours} \\ 1; & v_i, v_j \text{ adjacent with diffrenet colours or } i = j \text{ \& } v_i \in C \\ 0; & \text{in all other cases} \end{cases} \quad (1)$$

Minimum covering chromatic energy (MCChE) of G is $E_{CCh}(G) = \sum_{i=1}^n |k_i|$, where $k_1, k_2, \dots, k_n$ are characteristic values of $A_{CCh}(G)$ with an

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average $\bar{k}$. The minimum absolute deviation covering chromatic energy (MADCChE) of G is represented as [3, 5, 6]

$$\mathbb{E}_{CCh}^M(G) = \sum_{i=1}^n |k_i - \bar{k}|. \quad (2)$$

The Minimum covering colouring energy [1, 4] depends on the selection of covering set $\mathbf{C}$ and hence the MADCCChE also depends on $\mathbf{C}$ and the colours used for colouring of vertices. If $C = \{v_1, v_2, \dots, v_k\}$ is the MC set and $c_1, c_2, \dots, c_n$ are eigen values of $A_{CCh}(G)$ with mean $\bar{c}$ and $P = \det A_{CCh}(G)$, then [4]

$$\begin{aligned} \sqrt{(|C| + 2(4m_1 + m_2 + m_3) + n(n-1)P^2) / n} &\leq \mathbb{E}_{CP}(G) \\ &\leq \sqrt{n(|C| + 2(4m_1 + m_2 + m_3))} \end{aligned}$$

2. Main Results

Theorem 1: For $n \geq 2$, the MADCCChE of a complete graph $\mathcal{K}_n$ is

$$\frac{(n-1)(n-2)}{n} + \sqrt{n^2 + 2n - 3}.$$

Proof: Let $\mathcal{K}_n$ be with vertex set $V = \{v_1, v_2, \dots, v_n\}$.

Then MC set = $\{v_1, v_2, \dots, v_{n-1}\}$ with chromatic number 'n'.

$$\text{Then the MCCh matrix } \mathbb{A}_{CCh}(\mathcal{K}_n) = \begin{pmatrix} 1 & 1 & 1 & & 1 & 1 \\ 1 & 1 & 1 & \dots & 1 & 1 \\ 1 & 1 & 1 & & & 1 \\ & \vdots & & \ddots & & \\ 1 & 1 & 1 & \dots & 1 & 0 \end{pmatrix}_{n \times n}$$

Then the characteristic equation (CE) $|\mathbb{A}_{CP}(\mathcal{K}_n) - k I| = 0$ is

$$(k)^{n-2}(k^2 - (n-1)k - (n-1)) = 0.$$

and spectrum is

$$\text{Spec}_{CCh}(k_n) = \begin{pmatrix} 0 & \frac{(\sqrt{n^2+2n-3})+(n-1)}{2} & \frac{-(\sqrt{n^2+2n-3})+(n-1)}{2} \\ n-2 & 1 & 1 \end{pmatrix}$$

Mean $\bar{k} = \frac{n-1}{n}$. The MADChE is computed as

$$\begin{aligned} \mathbb{E}_{CCh}^M(\mathcal{K}_n) &= \sum_{i=1}^{n-2} \left| 0 - \frac{-1+n}{n} \right| + \left| \frac{(n-1) \pm \sqrt{2n+n^2-3}}{2} - \frac{-1+n}{n} \right| \\ &= \frac{(n-2)}{n} + \left| \frac{(n^2-3n+2) \pm \sqrt{2n+n^2-3}}{2n} \right| = \frac{(n-1)(n-2)}{n} + \sqrt{n^2 + 2n - 3}. \end{aligned}$$

Theorem 2: For $n \geq 3$, the MADCCChE of star graph $\mathcal{K}_{1,n-1}$ is

$$\frac{(n-2)(n+5)}{n} + \sqrt{n^2 + 2n - 3}.$$

Proof: Let $\mathcal{K}_{1,n-1}$ be with $V = \{v_1, v_2, \dots, v_n\}$.

The MC set = $\{v_1\}$ (where v_1 is the centre vertex) and $\chi(\mathcal{K}_{1,n-1}) = 2$.

Hence, the MCCh matrix of $\mathcal{K}_{1,n-1}$ is $\mathbb{A}_{CCh}(\mathcal{K}_{1,n-1})$

$$= \begin{pmatrix} 1 & 1 & 1 & & 1 & 1 \\ 1 & 0 & -1 & \cdots & -1 & -1 \\ 1 & -1 & 0 & & -1 & -1 \\ & \vdots & & \ddots & & \vdots \\ 1 & -1 & -1 & \cdots & 0 & \end{pmatrix}_{n \times n}$$

The CE $|\mathbf{A}_{CCh}(\mathcal{K}_{1,n-1}) - k \mathbf{I}| = 0$ is $(k-1)^{n-2}(c^2 + (n-3)c - (2n-3)) = 0$.

The spectrum of MCCh matrix of $k_{1,n-1}$ is

$$Spec_{CCh}(k_{1,n-1}) = \begin{pmatrix} 1 & \frac{(\sqrt{n^2+2n-3})+(n-3)}{2} & \frac{-(\sqrt{n^2+2n-3})+(n-3)}{2} \\ n-2 & 1 & 1 \end{pmatrix}$$

Mean $\bar{c} = \frac{2n-5}{n}$. The MADCCHE is computed as

$$\begin{aligned} \mathbb{E}_{CP}^M(\mathcal{K}_n) &= \sum_{i=1}^{n-2} \left| 1 - \frac{2n-5}{n} \right| + \left| \frac{(n-3) \pm \sqrt{n^2+2n-3}}{2} - \frac{-5+2n}{n} \right| \\ &= \frac{(n-2)(5+n)}{n} + \left| \frac{(n^2-7n+10) \pm n\sqrt{n^2+2n-3}}{2n} \right| \\ &= \frac{(n-2)(5+n)}{n} + \sqrt{n^2+2n-3}. \end{aligned}$$

Theorem 3: When $n \geq 3$, the MADCCPE for a Crown graph S_n^0 is $(n-1)\sqrt{5} + \sqrt{4n^2 - 10n + 13}$

Proof: Let $V = \{u_1, u_2, \dots, u_n, v_1, v_2, \dots, v_n\}$ be the vertex of a crown graph S_n^0 .

Then MC set $= \{u_1, u_2, \dots, u_n\}$ and $\chi(S_n^0) = 2$. Then MCCh matrix is an $2n \times 2n$ matrix

$$A_{CCh}(S_n^0) = \begin{bmatrix} 1 & -1 & -1 & . & . & -1 & 0 & 1 & . & . & 1 & 1 \\ -1 & 1 & -1 & . & . & -1 & 1 & 0 & . & . & 1 & 1 \\ -1 & -1 & 1 & . & . & -1 & 2 & 2 & . & . & -1 & -1 \\ . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . \\ -1 & -1 & -1 & . & . & 1 & 1 & 1 & . & . & 1 & 0 \\ 0 & 1 & 1 & . & . & 1 & 0 & -1 & . & . & -1 & -1 \\ 1 & 0 & 1 & . & . & 1 & -1 & 0 & . & . & -1 & -1 \\ . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . \\ 1 & 1 & 1 & . & 0 & 1 & -1 & -1 & . & . & 0 & -1 \\ 1 & 1 & 1 & . & . & 0 & -1 & -1 & . & . & -1 & 0 \end{bmatrix}$$

Then the CE $|\mathbf{A}_{CCh}(S_n^0) - k \mathbf{I}| = 0$ is

$$(k^2 - 3k + 1)^{n-1} (c^2 + (2n-3)c - (n-1)) = 0.$$

The spectrum of MCCh matrix of S_n^0 is

$$Spec_{CCh}(S_n^0) = \begin{pmatrix} \frac{3+\sqrt{5}}{2} & \frac{3-\sqrt{5}}{2} & \frac{(-2n+3)+\sqrt{4n^2-10n+13}}{2} & \frac{(-2n+3)-\sqrt{4n^2-10n+13}}{2} \\ n-1 & n-1 & 1 & 1 \end{pmatrix}$$

Mean $\bar{k} = \frac{1}{2}$. Then MADCCChE of crown graph

$$E_{CCh}^M(S_n^0) = \sum_{i=1}^{n-1} \left| \left(\frac{3 \pm \sqrt{5}}{2} - \frac{1}{2} \right) \right| + \left| \frac{(-2n+3) \pm \sqrt{4n^2-10n+13}}{2} - \frac{1}{2} \right| \\ = (n-1) \sqrt{5} + \sqrt{4n^2-10n+13}.$$

Theorem 4: The MADCCChE of the complete bipartite graph $\mathcal{K}_{m,n}$ with vertices

$$(n+m) \text{ is } \frac{m^2+2mn-3n+n^2-m}{m+n} + \sqrt{m^2+2mn+2n+n^2-2m+1}$$

Proof: For partite sets $V_1 = \{u_1, u_2, \dots, u_m\}$, $V_2 = \{v_1, v_2, \dots, v_n\}$ of $\mathcal{K}_{m,n}$, with $|n-m| > 1$, $n \geq 2$ & $m \geq 2$, having vertices $V = (V_1, V_2)$, the MC is $C = \{u_1, u_2, \dots, u_m\}$ and chromatic number is equal to 2. The MC set = $\{u_1, u_2, \dots, u_m\}$. Hence, the MCCh matrix is $A_{CCh}(\mathcal{K}_{m,n})$

$$= \begin{bmatrix} 1 & -1 & -1 & . & . & -1 & 1 & 1 & 1 & . & 1 & 1 \\ -1 & 1 & -1 & . & . & -1 & 1 & 1 & 1 & . & 1 & 1 \\ -1 & -1 & 1 & . & . & -1 & 1 & 1 & 1 & . & 1 & 1 \\ . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . \\ -1 & -1 & -1 & . & . & 1 & 1 & 1 & 1 & . & 1 & 1 \\ 1 & 1 & 1 & . & . & 1 & 0 & -1 & -1 & . & -1 & -1 \\ 1 & 1 & 1 & . & . & 1 & -1 & 0 & -1 & . & -1 & -1 \\ 1 & 1 & 1 & . & . & 1 & -1 & -1 & 0 & .. & -1 & -1 \\ 1 & 1 & 1 & . & . & 1 & -1 & -1 & -1 & 0.. & -1 & -1 \\ . & . & . & . & . & . & . & . & . & . & . & . \\ 1 & 1 & 1 & . & . & 1 & -1 & -1 & -1 & . & -1 & 0 \end{bmatrix}$$

Then the CE $|A_{CCh}(\mathcal{K}_{m,n}) - k I| = 0$ is

$$(-k+1)^{n-1}(k-2)^{m-1}(k^2+(n+m-3)k-(m+2n-2))=0.$$

The spectrum of MCCh matrix of $\mathcal{K}_{n,n}$ is $Spec_{CCh}(\mathcal{K}_{n,n})$

$$= \left(\begin{array}{cc} 1 & 2 \\ n-1 & m-1 \end{array} \begin{array}{c} ((3-n-m)+\sqrt{2nm+m^2+2n-2m+1})/2 \\ 1 \end{array} \right. \\ \left. \begin{array}{c} ((3-m-n)+\sqrt{m^2+2mn+2n-2m})/2 \\ 1 \end{array} \right)$$

Mean $\bar{k} = \frac{m}{m+n}$. The MADCCChE is computed as

$$E_{CCh}^M(\mathcal{K}_{n,n}) = \sum_{i=1}^{n-1} \left| \left(1 - \frac{m}{m+n} \right) \right| + \sum_{i=1}^{m-1} \left| \left(2 - \frac{m}{m+n} \right) \right| \\ + \left| \frac{(3-n-m) \pm \sqrt{m^2+2mn+2n+n^2+1-2m}}{2} - \frac{m}{m+n} \right| \\ = \frac{(n-1)n}{m+n} + \frac{(m+2n)(m-1)}{m+n} + \\ + \left| \frac{(m+3n)-(m+n)^2 \pm (m+n)\sqrt{m^2+2mn+2n+n^2-2m+1}}{2(m+n)} \right| \\ = \frac{m^2+2mn-3n+n^2-m}{m+n} + \sqrt{m^2+2mn+2n+n^2-2m+1}$$

Theorem 5: For $n \geq 3$, the MADCCChE for a cocktail party graph $\mathcal{K}_{n \times 2}$ equals to $\frac{4n^2-7n+1}{n} + \sqrt{4n^2 + 14n - 7}$.

Proof: For $\mathcal{K}_{n \times 2}$ with $V = \cup_{i=1}^n \{u_i, v_i\}$, the MC set is $C = \cup_{i=1}^{n-1} \{u_i, v_i\}$ and $\chi(\mathcal{K}_{n \times 2}) = n$ so that $c(u_i) = C(v_i)$

Hence, the MCCCh matrix is

$$A_{CCh}(\mathcal{K}_{n \times 2}) = \begin{bmatrix} 1 & -1 & 1 & 1 & . & . & . & . & 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 & . & . & . & . & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & . & . & . & . & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & . & . & . & . & 1 & 1 & 1 & 1 \\ . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . & . & . & . \\ 1 & 1 & 1 & 1 & . & . & . & . & 1 & 1 & 0 & -1 \\ 1 & 1 & 1 & 1 & . & . & . & . & 1 & 1 & -1 & 0 \end{bmatrix}$$

Then the CE is

$$(k-1)(k+2)^{-2+n}(2-k)^{-1+n}(k^2 - (2n-5)k - (6n-8)) = 0.$$

The spectrum of MCCCh matrix of $\mathcal{K}_{m,n}$ is $Spec_{CCh}(\mathcal{K}_{n \times 2})$

$$= \left(\begin{array}{cccc} -2 & 2 & 1 & \frac{(2n-5)+\sqrt{4n^2+14n-7}}{2} & \frac{(2n-5)-\sqrt{4n^2+14n-7}}{2} \\ n-2 & n-1 & 1 & 1 & 1 \end{array} \right)$$

Mean $\bar{k}$ is $\frac{n-1}{n}$. The MADCCChE is computed as

$$\begin{aligned} \mathbb{E}_{CCh}^M(\mathcal{K}_{n \times 2}) &= \sum_{i=1}^{n-2} \left| \left(-2 - \frac{n-1}{n} \right) \right| + \sum_{i=1}^{n-1} \left| \left(-\frac{n-1}{n} + 2 \right) \right| + \left| 1 + \frac{1-n}{n} \right| \\ &\quad + \left| \frac{(2n-5) \pm \sqrt{4n^2+14n-7}}{2} - \frac{n-1}{n} \right| \\ &= \frac{4n^2-7n+1}{n} + \sqrt{4n^2 + 14n - 7}. \end{aligned}$$

Similarly, we can calculate for other graphs.

Theorem 6: If $C = \{v_1, v_2, \dots, v_k\}$ is the MC set and $c_1, c_2, \dots, c_n$ are eigen values of $A_{CCh}(G)$ with mean $\bar{c}$ and $P = \det A_{CCh}(G)$, then

- (i) $\sum_{i=1}^n c_i = |C|$
- (ii) $\sum_{i=1}^n c_i^2 = 2m + k + 2M$, where $m = |E|$ and the quantity of pairs of non-adjacent vertices exhibiting identical coloration in the graph G is denoted as M .

Proof:

- (i) Result follows as sum of eigen values of $A_{CCh}(G)$ is nothing but its trace.
- (ii) Result follows as (i)

Theorem 7: If $C = \{v_1, v_2, \dots, v_k\}$ is the MC set and $c_1, c_2, \dots, c_n$ are eigen values of $A_{CCh}(G)$ with mean $\bar{c}$ and $P = \det A_{CCh}(G)$, then

$$\sqrt{(|C| + 2m + 2M) - 2|\bar{c}| \sqrt{(2m + |C| + 2M)n}} \leq \mathbb{E}_{CCh}^M(G) \leq \sqrt{(2m + |C| + n\bar{c}^2 + 2M)n}.$$

Proof: By Cauchy Schwarz inequality $(\sum_{i=1}^n |a_i b_i|)^2 = (\sum_{i=1}^n a_i^2) (\sum_{i=1}^n b_i^2)$

Take $a_i = 1$, $b_i = |c_i - \bar{c}|$ then,

$$\begin{aligned} [\mathbb{E}_{CCh}^M(G)]^2 &= (\sum_{i=1}^n 1) (\sum_{i=1}^n |c_i - \bar{c}|^2) \\ &= (n) (\sum_{i=1}^n |c_i - \bar{c}|^2) \leq n (\sum_{i=1}^n c_i^2 + \sum_{i=1}^n \bar{c}^2) \\ &= n (\sum_{i=1}^n c_i^2 + n\bar{c}^2) = n(|C| + 2m + 2M + n\bar{c}^2) \end{aligned}$$

Then

$$\mathbb{E}_{CCh}^M(G) \leq \sqrt{n(2m + |C| + n\bar{c}^2 + 2M)}$$

Also

$$\begin{aligned} [\mathbb{E}_{CCh}^M(G)]^2 &= (\sum_{i=1}^n |c_i - \bar{c}|)^2 \\ &\geq \sum_{i=1}^n |c_i - \bar{c}|^2 \geq \sum_{i=1}^n |c_i|^2 - 2|\bar{c}| \sum_{i=1}^n |c_i| \\ &\geq (2m + |C| + 2M) - 2|\bar{c}| \sqrt{n(|C| + 2m + 2M)} \end{aligned}$$

Then

$$\mathbb{E}_{ED}^M(G) \geq \sqrt{(|C| + 2M + 2m) - 2|\bar{c}| \sqrt{n(2M + |C| + 2m)}}$$

Hence the theorem.

3. Conclusion

The absolute deviation covering partition energy (ADCCHE) for various graph structures, including the complete graph, cocktail party graph, complete bipartite graph, crown graph, and star graph has been computed. Furthermore, the established lower and upper bounds of the absolute deviation covering partition energy have been delineated. This theoretical framework can be extrapolated to encompass alternate standard graphs as well as their corresponding complements.

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