Recent Results on the Irregularity and the Mostar Index of Graphs

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Joint with Štefko Miklavič, Johannes Pardey, Florian Werner

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ORIGINAL PAPER



Mostar index

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The Mostar index Mo(G) of a graph G is

$$Mo(G) = \sum_{uv \in E(G)} |n_G(u,v) - n_G(v,u)|,$$

where, for an edge uv of G,

 $n_G(u, v)$ is the number of vertices of G with smaller distance in G to u than to v,

that is,

$$n_G(u,v) = |\{w \in V(G) : \operatorname{dist}_G(u,w) < \operatorname{dist}_G(v,w)\}|.$$

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$$n_G(u,v) = \big| \big\{ w \in V(G) : \operatorname{dist}_G(u,w) < \operatorname{dist}_G(v,w) \big\} \big|.$$

• Since $|n_G(u, v) - n_G(v, u)| \le (n - 1) - 1 = n - 2$, we have

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$$n_G(u,v) = \big| \big\{ w \in V(G) : \operatorname{dist}_G(u,w) < \operatorname{dist}_G(v,w) \big\} \big|.$$

• Since $|n_G(u, v) - n_G(v, u)| \le (n - 1) - 1 = n - 2$, we have $Mo(G) \le m(n - 2) < 0.5n^3$.

• G is distance-balanced if $n_G(u, v) = n_G(v, u)$ for every edge uv of G.

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Mostar index: Results and perspectives



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ABSTRACT

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05C09	
05C12	
05C92	

The Mostar index is a recently introduced bond-additive distance-based graph invariant that measures the degree of peripherality of particular edges and of the graph as a whole. It attracted considerable attention, both in the context of complex networks and in more classical applications of chemical graph theory, where it turned out to be useful as a measure of the total surface area of octane isomers and as a tool for studying topological aspects of fullerene shapes. This paper aims to gather some known bounds and extremal results concerning the Mostar index. Also, it presents various modifications and generalizations of the aforementioned index and it outlines several possible directions of further research. Finally, some open problems and conjectures are listed.

[1]-[78], sparse graphs and trees, chemical graphs, hypercube-related graphs

Relation to the Wiener index

The Wiener index W(G) of a graph G [Wiener 1947] is

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} \left(\sum_{v \in V(G)} \operatorname{dist}_{G}(u, v) \right)$$
$$= \frac{1}{2} \sum_{u \in V(G)} \sigma_{G}(u).$$

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$$\begin{split} \mathcal{W}(G) &= \frac{1}{2} \sum_{u \in V(G)} \left(\sum_{v \in V(G)} \operatorname{dist}_{G}(u, v) \right) \\ &= \frac{1}{2} \sum_{u \in V(G)} \sigma_{G}(u). \end{split}$$

Since

$$|n_G(u,v) - n_G(v,u)| = |\sigma_G(u) - \sigma_G(v)|$$
 for every edge uv of G ,

we have

$$Mo(G) = \sum_{uv \in E(G)} |\sigma_G(u) - \sigma_G(v)|.$$

Relation to the irregularity

The irregularity irr(G) of a graph G [Albertson 1997] is

$$\operatorname{irr}(G) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)|.$$

Relation to the irregularity

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If $diam(G) \leq 2$, then



$$|n_G(u, v) - n_G(v, u)| = |(a+1) - (c+1)|$$

= |(a+b+1) - (b+c+1)|
= |d_G(u) - d_G(v)|,

and, hence,

$$Mo(G) = \operatorname{irr}(G)$$

5.2 Conjectures and open problems

For the beginning, it would be interesting to investigate how the results of papers concerned with distance-balanced graphs extend to the case Mo (G) $\neq 0$.

We have already mentioned that Mo $(K_{\lfloor n/3 \rfloor, \lceil 2n/3 \rceil}) \sim 2n^3/27 \in \Theta(n^3)$. We believe that this is the extremal graph among all bipartite graphs on the same number of vertices.

Conjecture 19 Among bipartite graphs on *n* vertices $K_{n/3,2n/3}$ has the maximal Mostar index.

For general graphs, the extremal graph is most likely the split graph with the same parameters. The *split graph* $S_{m,n}$ is obtained by taking a complete graph K_m on m vertices and n isolated vertices $\overline{K_n}$ and connecting every isolated vertex to all vertices of K_m . A split graph is a join of a complete graph and the complement of another complete graph.

Conjecture 20 Among all graphs on *n* vertices the split graph $S_{n/3,2n/3}$ has the maximal Mostar index.

As observed by Geneson and Tsai [2021], for $\alpha \leq \frac{1}{2}$,

$$Mo(K_{\alpha n,(1-\alpha)n}) = \alpha n(1-\alpha)n(1-2\alpha)n = \alpha(1-\alpha)(1-2\alpha)n^{3}$$

and

$$\underset{\alpha}{\operatorname{argmax}} \alpha(1-\alpha)(1-2\alpha) = \frac{1}{2}\left(1-\frac{1}{\sqrt{3}}\right) =: \alpha^{\star} \approx 0.21132.$$

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Hence, at least for large n,

$$Mo(K_{0.211...n,0.789...n}) > Mo(K_{0.\overline{3}n,0.\overline{6}n}),$$

and Conjecture 19 cannot hold as stated.

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Albertson [1997] showed

$$\operatorname{irr}(G) \leq \frac{4}{27}n^3,$$

which implies Conjecture 20 up to $O(n^2)$ provided that diam $(G) \leq 2$.

Theorem (MPRW 2022)

If G is a bipartite graph of order n, then

$$Mo(G) \leq \alpha^{\star}(1-\alpha^{\star})(1-2\alpha^{\star})n^{3} = \frac{\sqrt{3}}{18}n^{3} \approx 0.096225n^{3}.$$

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which implies

$$|n_G(u, v) - n_G(v, u)| \leq n - 2\min\{d_G(u), d_G(v)\} \\ = n\left(1 - \frac{2}{n}\min\{d_G(u), d_G(v)\}\right).$$

We obtain

$$Mo(G) \leq \sum_{uv \in E(G)} n\left(1 - \frac{2}{n}\min\left\{d_G(u), d_G(v)\right\}\right),$$

and we show the stated bound for the right hand side.

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• Let the partite sets V_1 and V_2 of G have orders αn and $(1 - \alpha)n$ for some $\alpha \in (0, 1/2]$.

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• Let
$$I = \{0, 1, \dots, (1 - \alpha)n\}$$
 and $J = \{0, 1, \dots, \alpha n\}$.

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- Let the partite sets V_1 and V_2 of G have orders αn and $(1 \alpha)n$ for some $\alpha \in (0, 1/2]$.
- Let $I = \{0, 1, \dots, (1 \alpha)n\}$ and $J = \{0, 1, \dots, \alpha n\}$.
- Let V_1 contain exactly $x_i \alpha n$ vertices of degree *i* for every $i \in I$.

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- Let V_1 contain exactly $x_i \alpha n$ vertices of degree *i* for every $i \in I$.
- Let V_2 contain exactly $y_i(1-\alpha)n$ vertices of degree j for every $j \in J$.

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- Let V_1 contain exactly $x_i \alpha n$ vertices of degree *i* for every $i \in I$.
- Let V_2 contain exactly $y_j(1-\alpha)n$ vertices of degree j for every $j \in J$.
- Let G have exactly $m_{i,j}\alpha(1-\alpha)n^2$ edges between a vertex from V_1 of degree i and a vertex from V_2 of degree j for every $(i,j) \in I \times J$.

Since
$$\sum_{j\in J} m_{i,j}\alpha(1-\alpha)n^2 = ix_i\alpha n$$
,

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$$\sum_{j\in J}m_{i,j}-rac{ix_i}{(1-lpha)n}=0$$
 for every $i\in I$,

and, symmetrically,

$$\sum_{i \in I} m_{i,j} - \frac{jy_i}{\alpha n} = 0 \text{ for every } j \in J.$$

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We obtain

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for the following linear programm (P):

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for the following linear programm (P):

$$\begin{array}{rcl} \max & \sum\limits_{(i,j)\in I\times J} m_{i,j} \left(1-\frac{2}{n}\min\{i,j\}\right),\\ s.th. & \sum\limits_{i\in I} x_i &=& 1,\\ & \sum\limits_{j\in J} y_j &=& 1,\\ & \sum\limits_{j\in J} m_{i,j} - \frac{ix_i}{(1-\alpha)n} &=& 0 \quad \text{for every } i\in I,\\ & \sum\limits_{i\in I} m_{i,j} - \frac{jy_j}{\alpha n} &=& 0 \quad \text{for every } j\in J,\\ & x_i, y_j, m_{i,j} &\geq& 0 \quad \text{for every } (i,j)\in I\times J. \end{array}$$

The dual of (P) is the following linear programm (D):

 $\begin{array}{rcl} \min & p+q, \\ s.th. & p_i+q_j & \geq & 1-\frac{2}{n}\min\{i,j\} & \text{ for every } i \in I \text{ and every } j \in J, \\ (D) & p & \geq & \frac{ip_i}{(1-\alpha)n} & \text{ for every } i \in I, \\ & q & \geq & \frac{jq_j}{\alpha n} & \text{ for every } j \in J, \\ & p,q,p_j,q_j & \in & \mathbb{R} & \text{ for every } i \in I \text{ and every } j \in J. \end{array}$

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• We just need weak duality $OPT(P) \le OPT(D)$.

•
$$p \stackrel{!}{=} \frac{ip_i}{(1-\alpha)n}$$
 for $i \ge 1 \Rightarrow p_i = \frac{(1-\alpha)n}{i}p$.

• $q_j = \frac{\alpha n}{j}q$ for $j \ge 1$.

$$p_i + q_j \ge 1 - \frac{2}{n} \min\{i, j\}$$
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$$\frac{p}{\left(\frac{i}{(1-\alpha)n}\right)} + \frac{2i}{n} + q \ge 1 \text{ for } 1 \le i \le \alpha n.$$

$$\uparrow$$

$$\left(\frac{p}{x} + 2(1-\alpha)x\right) + q \ge 1 \quad \text{for} \quad x = \frac{i}{(1-\alpha)n} \in \left(0, \frac{\alpha}{1-\alpha}\right].$$
Bipartite graphs



For some $\delta > 0$, the function

$$f:(0,\infty)\to\mathbb{R}:x\mapsto rac{\beta}{x}+\gamma x$$

with $\beta \geq 0$ and $\gamma > 0$ satisfies

$$\min \left\{ f(x) : x \in (0, \delta] \right\} = \begin{cases} f\left(\sqrt{\frac{\beta}{\gamma}}\right) = 2\sqrt{\beta\gamma} & \text{, if } \delta \ge \sqrt{\frac{\beta}{\gamma}}, \\ f(\delta) & \text{, if } \delta \le \sqrt{\frac{\beta}{\gamma}}. \end{cases}$$

Bipartite graphs

It follows $\operatorname{OPT}(D) \leq \operatorname{OPT}(D')$ for

	min	p+q,			
	s.th.	p+q	\geq	1-2lpha,	
(D')		$p + 2\sqrt{2q\alpha}$	\geq	1	$\text{ if } \textbf{\textit{q}} < 2\alpha,$
		$2\sqrt{2p(1-lpha)}+q$	\geq	1	if $p < \frac{2\alpha^2}{1-\alpha}$
		p, q	\geq	0.	

Bipartite graphs

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 $\begin{array}{rll} \min & p+q, \\ s.th. & p+q \geq 1-2\alpha, \\ (D') & p+2\sqrt{2q\alpha} \geq 1 & \text{if } q < 2\alpha, \\ & 2\sqrt{2p(1-\alpha)}+q \geq 1 & \text{if } p < \frac{2\alpha^2}{1-\alpha}, \\ & p,q \geq 0. \end{array}$

The proof is now completed by showing

$$OPT(D') \le \frac{\alpha^*(1-\alpha^*)(1-2\alpha^*)}{\alpha(1-\alpha)}.$$

Theorem (MPRW 2022)

If G is a split graph that arises from a clique C of order αn and an independent set I of order $(1 - \alpha)n$ for some $\alpha \in [0, 1]$ by adding m edges between vertices in C and vertices in I,

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If G is a split graph that arises from a clique C of order αn and an independent set I of order $(1 - \alpha)n$ for some $\alpha \in [0, 1]$ by adding m edges between vertices in C and vertices in I, then

$$\begin{aligned} \mathsf{Mo}(G) &\leq ((1+\alpha)n-1)m - \frac{2m^2}{(1-\alpha)n} \\ &\leq \begin{cases} \alpha(1-\alpha)n^2\Big((1-\alpha)n-1\Big) &, \text{ if } \alpha \leq \frac{1}{3} - \frac{1}{3n}, \\ \frac{1}{8}(1-\alpha)n\Big((1+\alpha)n-1\Big)^2 &, \text{ if } \alpha > \frac{1}{3} - \frac{1}{3n} \\ &\leq \frac{4}{27}n^3. \end{aligned}$$

Each stated bound is best possible up to $O(n^2)$.

Let G be as in the statement and let uv be an edge of G.

$$|n_G(u,v) - n_G(v,u)| \leq \begin{cases} n - d_G(v) - 1 & \text{, if } u \in C \text{ and } v \in I, \\ |d_G(u) - d_G(v)| & \text{, if } u, v \in C. \end{cases}$$

Let E be the set of the m edges of G between C and I.

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Let E be the set of the m edges of G between C and I.

$$\begin{aligned} \mathsf{Mo}(G) &\leq \sum_{uv \in E} (n - d_G(v) - 1) + \sum_{uv \in \binom{C}{2}} |d_G(u) - d_G(v)| \\ &= m(n - 1) - \sum_{v \in I} d_G(v)^2 + \sum_{uv \in \binom{C}{2}} |d_G(u) - d_G(v)| \\ &\leq m(n - 1) - \frac{m^2}{(1 - \alpha)n} + \sum_{uv \in \binom{C}{2}} |d_G(u) - d_G(v)| \\ &\leq m(n - 1) - \frac{m^2}{(1 - \alpha)n} + \alpha nm - \frac{m^2}{(1 - \alpha)n} \end{aligned}$$

General graphs Conjecture 20 would imply

$$Mo(G) \leq rac{4}{27}n^3 = 0.\overline{148}n^3.$$

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Geneson and Tsai [2021] improved $Mo(G) < 0.5n^3$ to

$$\begin{aligned} \mathsf{Mo}(G) &\leq \mathsf{Mo}^{\star}(G) &:= \sum_{uv \in E(G)} \underbrace{(n - \min\{d_G(u), d_G(v)\})}_{&\geq |n_G(u,v) - n_G(v,u)|} \\ &\leq \frac{5}{24} (1 + o(1)) n^3 \approx 0.2083 (1 + o(1)) n^3. \end{aligned}$$

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Adapting the linear programming approach yields...

Theorem (MPRW 2022)

If G is a graph of order n and maximum degree $\Delta,$ then

$$Mo^{\star}(G) \leq \left(2\left(\frac{\Delta}{n}\right)^2 + \left(\frac{\Delta}{n}\right) - 2\left(\frac{\Delta}{n}\right)\sqrt{\left(\frac{\Delta}{n}\right)^2 + \left(\frac{\Delta}{n}\right)}\right) n^3 \leq \left(3 - 2\sqrt{2}\right)n^3 \approx 0.1716n^3.$$

Theorem (MPRW 2022)

If G is a graph of order n, then
$$Mo^{\star}(G) \leq \left(\frac{2}{\sqrt{3}} - 1\right)n^3 \leq 0.1548n^3$$
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The proof is by induction in n.

n = 1: Trivial.

n > 1: Let the graph G of order n be such that

(i) $Mo^*(G)$ is as large as possible,

(ii) subject to (i), the graph G has as many edges as possible, and

(iii) subject to (i) and (ii), the term $\sum_{u \in V(G)} d_G^2(u)$ is as large as possible.

Theorem (MPRW 2022)

If G is a graph of order n, then
$$Mo^{\star}(G) \leq \left(rac{2}{\sqrt{3}}-1
ight)n^3 \leq 0.1548n^3.$$

The proof is by induction in n.

n = 1: Trivial.

n > 1: Let the graph G of order n be such that

(i) $Mo^*(G)$ is as large as possible,

(ii) subject to (i), the graph G has as many edges as possible, and

(iii) subject to (i) and (ii), the term $\sum_{u \in V(G)} d_G^2(u)$ is as large as possible.

There is a linear ordering $\pi : u_1, u_2, \ldots, u_n$ of V(G) such that

$$d_G(u_1) \leq d_G(u_2) \leq \ldots \leq d_G(u_n)$$

and

$$d_1^+ \geq d_2^+ \geq \ldots \geq d_n^+,$$

where d_i^+ be the number of forward edges at u_i .

• u1

• · · · · • u_1 $u_{n-\delta}$

•	 •
<i>u</i> ₁	$u_{n-\delta}$

	1	
•		•
<i>u</i> 1		$u_{n-\delta}$













 $n - \min\{d_G(u), d_G(v)\} = \delta - \min\{d_H(u), d_H(v)\}$ for every edge uv of H



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$$Mo^{\star}(G) = \delta(n-\delta)^2 + Mo^{\star}(H) \stackrel{I}{\leq} \delta(n-\delta)^2 + \left(\frac{2}{\sqrt{3}}-1\right)\delta^3 \leq \left(\frac{2}{\sqrt{3}}-1\right)n^3.$$

Albertson [1997] defined the irregularity irr(G) of a graph G as

$$irr(G) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)|.$$

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$$irr(G) \leq \max_{p} S_{p,n-p} = \left\lfloor \frac{n}{3} \right\rfloor \left\lceil \frac{2n}{3} \right\rceil \left(\left\lceil \frac{2n}{3} \right\rceil - 1 \right) < \frac{4n^3}{27}$$

Hansen and Mélot [2005]

 $irr(G) \leq f(n,m)$

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For a graph G with n vertices, m edges, maximum degree Δ , and minimum degree δ , Zhou and Luo [2008] showed

$$irr(G) \leq m\sqrt{\frac{2n\left(2m+(n-1)(\Delta-\delta)\right)}{n+\Delta-\delta}-4m}$$
 and
 $irr(G) \leq \sqrt{m\left(2mn(\Delta+\delta)-n^2\Delta\delta-4m^2\right)},$

Using variations of $S_{p,n-p}$, Abdo, Cohen, and Dimitrov [2014] provided lower bounds on the maximum irregularity of graphs of given order, maximum degree, and minimum degree.

- Bipartite graphs [Henning and Rautenbach 2007]
- Bounded clique number [Zhou and Luo 2008]
- Graphs with a given number of vertices of degree 1 [Dorjsembe, Buyantogtokh, Das, and Horoldagva 2022] [Liu, Chen, Hu, and Zhu 2022]

$$K_1, K_{\Delta,1}, K_{\Delta,2}, K_{\Delta,3}, K_{\Delta,4}, \ldots, K_{\Delta,\Delta-1}, K_{\Delta,\Delta}$$

Theorem (RW 2023)

Let G be a graph with n vertices, m edges, and maximum degree at most Δ , where Δ is a positive integer. If $d \in \{0, ..., \Delta - 1\}$ is such that $\frac{2m}{n} \in \left[\frac{2\Delta d}{\Delta + d}, \frac{2\Delta(d+1)}{\Delta + d+1}\right]$, then

$$irr(G) \leq d(d+1)n + rac{1}{\Delta} \left(\Delta^2 - (2d+1)\Delta - d^2 - d\right)m.$$

 $(\textit{n},\Delta) \in \{(60,3),(100,10)\}$



Corollary (RW 2023)

If G is a graph with n vertices, m edges, and maximum degree at most Δ , where Δ is a positive integer, then

$$\operatorname{irr}(G) \leq rac{(\Delta n - 2m)\Delta m}{\Delta n - m} < rac{\left(2 - \sqrt{2}\right)\left(\sqrt{2} - 1
ight)}{\sqrt{2}}\Delta^2 n.$$



Comparing to Zhou and Luo [2008]:



For integers $\Delta > \delta \ge 0$, let

$$\begin{split} \delta^* &= \operatorname{argmax} \left\{ \frac{\Delta \left(\Delta - i\right) i}{\Delta + i} : i \in \{\delta, \dots, \Delta\} \right\} \\ &\in \left\{ \begin{cases} \left\lfloor \left(\sqrt{2} - 1\right) \Delta \right\rfloor, \left\lceil \left(\sqrt{2} - 1\right) \Delta \right\rceil \right\}, & \text{if } \delta \leq \left\lfloor \left(\sqrt{2} - 1\right) \Delta \right\rfloor \\ \\ \left\{\delta\}, & \text{otherwise.} \end{cases} \end{split} \right.$$

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Proposition (RW 2023)

If G is a graph with n vertices, maximum degree at most Δ , and minimum degree at least δ , where $\Delta > \delta \ge 0$ are integers, and δ^* is as above, then

$$irr(G) \leq rac{\Delta \left(\Delta - \delta^*\right) \delta^*}{\Delta + \delta^*} n_{\bullet}$$

Proposition (RW 2023)

Let G be a graph with n vertices, m edges, maximum degree at most Δ , and minimum degree at least δ , where $\Delta > \delta \ge 1$ are integers. If $\frac{2m}{n} \in \left[\delta, \frac{2\Delta\delta}{\Delta+\delta}\right]$, then

 $irr(G) \leq 2\Delta m - \delta \Delta n.$

 $(n, \Delta, \delta) = (50, 10, 4), \ m \in [100, 250]$



Let $I_0 = \{0, 1, \dots, \Delta\}$ and $I = I_0 \setminus \{0\}$.

 $irr(G) \leq OPT(P)$

$$\max \sum_{\substack{i,j \in I: i < j}} (j-i)m_{i,j}$$
s.th.

$$\sum_{\substack{i,j \in I: i < j}} n_i = n,$$

$$\sum_{\substack{i \in I_0}} in_i = 2m,$$

$$2m_{i,i} + \sum_{j \in I: j < i} m_{j,i} + \sum_{\substack{j \in I: j > i}} m_{i,j} - in_i = 0 \quad \text{for every } i \in I,$$

$$n_i \in \mathbb{R}_{\ge 0} \quad \text{for every } i \in I_0, \text{ and}$$

$$m_{i,j} \in \mathbb{R}_{\ge 0} \quad \text{for every } i, j \in I \text{ with } i \le j.$$

$$(D) \qquad \begin{array}{ll} \min & nx + 2my \\ s.th. & z_i + z_j & \geq & j - i \quad \text{ for every } i, j \in I \text{ with } i < j, \\ (D) & x + iy & \geq & iz_i \quad \text{ for every } i \in I, \\ & x \quad \in \quad \mathbb{R}_{\geq 0}, \\ & y \quad \in \quad \mathbb{R}, \quad \text{ and} \\ & z_i \quad \in \quad \mathbb{R}_{>0}, \quad \text{ for every } i \in I. \end{array}$$

$$(D) \qquad \begin{array}{lll} \min & nx + 2my \\ s.th. & z_i + z_j & \geq & j - i & \text{ for every } i, j \in I \text{ with } i < j, \\ (D) & x + iy & \geq & iz_i & \text{ for every } i \in I, \\ & x & \in & \mathbb{R}_{\geq 0}, \\ & y & \in & \mathbb{R}, & \text{ and} \\ & z_i & \in & \mathbb{R}_{\geq 0}, & \text{ for every } i \in I. \end{array}$$

$$\sum_{\substack{i,j \in I: i < j \\ i,j \in I: i < j}} (j-i)m_{i,j}$$

$$\leq \sum_{\substack{i,j \in I: i < j \\ i=j-i}} (\underline{z_i + z_j})m_{i,j} + 2 \sum_{i \in I} z_i m_{i,i} + xn_0 + \sum_{i \in I} (x + iy - iz_i)n_i$$

$$\geq 0$$

$$= \left(\sum_{i \in I_0} n_i\right) x + \left(\sum_{i \in I} in_i\right) y + \sum_{i \in I} \left(2m_{i,i} + \sum_{j \in I: j < i} m_{j,i} + \sum_{j \in I: j > i} m_{i,j} - in_i\right) z_i$$

$$= nx + 2my.$$

 $(x, y, (z_i)_{i \in I})$ with

$$\begin{array}{rcl} x & = & d(d+1), \\ y & = & \displaystyle \frac{1}{2\Delta} \left(\Delta^2 - (2d+1)\Delta - d^2 - d \right), \text{ and} \\ z_i & = & \displaystyle \frac{1}{i} x + y \text{ for } i \in I \end{array}$$

is a feasible solution for (D).

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is a feasible solution for (D).

$$\begin{array}{ll} \operatorname{irr}(G) &\leq & \operatorname{OPT}(P) \\ &\leq & \operatorname{OPT}(D) \\ &\leq & \operatorname{nx} + 2my \\ &= & d(d+1)n + \frac{1}{\Delta} \left(\Delta^2 - (2d+1)\Delta - d^2 - d \right) m, \end{array}$$

3012

Journal of Mathematical Chemistry (2018) 56:2995–3013

Problem 21 Find chemical graphs and chemical trees on n vertices with largest Mostar index.

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- Chemical trees [Deng and Li 2021]
- Trees with given degree sequence [Deng and Li 2021]

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Problem 21 Find chemical graphs and chemical trees on n vertices with largest Mostar index.

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$$Mo(G) \leq m(n-2) \leq \frac{\Delta}{2}n(n-2) = \frac{\Delta}{2}n^2 - c_{\Delta}n^2$$

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$$Mo(G) \leq m(n-2) \leq \frac{\Delta}{2}n(n-2) = \frac{\Delta}{2}n^2 - c_{\Delta}n.$$

We conjecture that

 $\max \{Mo(G) : G \text{ has order } n \text{ and maximum degree at most } \Delta\}$

is

$$\frac{\Delta}{2}n^2 - \Theta_{\Delta}(n\log(n)).$$

Theorem (HPRW 2023)

For integers n_0 and Δ at least 3, there is a Δ -regular graph G of order n at least n_0 with

$$Mo(G) \geq \frac{\Delta}{2}n^2 - (20\Delta^3 + 12\Delta^2 - 24\Delta + 48) n \log_{(\Delta-1)}(n).$$

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ight) n \log_{(\Delta-1)}(n).$$

Theorem (HPRW 2023)

For integers n and Δ at least 3, if G is a graph of order n and maximum degree at most Δ , then

$$Mo(G) \leq \frac{\Delta}{2}n^2 - (2 - o(n))\frac{(\Delta - 2)}{(\Delta - 1)^2}n\log_{(\Delta - 1)}\left(\log_{(\Delta - 1)}(n)\right).$$



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A problem from [Doslic et al. 2018]



A problem from [Doslic et al. 2018]



 $|n_G(u, v) - n_G(v, u)| \le n - 2\min\{p, q\}$

A problem from [Doslic et al. 2018]



$$|n_G(u,v) - n_G(v,u)| \leq n - 2\min\{p,q\}$$
$$\sum_{uv \in E(T)} \min\{p,q\} \geq (1 - o(n))c_{\Delta}n\log(\log(n)).$$

Thank you for the attention!

