# 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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## Mostar index

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## ORIGINAL PAPER

## Mostar index

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## Mostar index

The Mostar index $\operatorname{Mo}(G)$ of a graph $G$ is

$$
M o(G)=\sum_{u v \in E(G)}\left|n_{G}(u, v)-n_{G}(v, u)\right|
$$

where, for an edge $u v$ 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,

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n_{G}(u, v)=\left|\left\{w \in V(G): \operatorname{dist}_{G}(u, w)<\operatorname{dist}_{G}(v, w)\right\}\right| .
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- Since $\left|n_{G}(u, v)-n_{G}(v, u)\right| \leq(n-1)-1=n-2$, we have

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M o(G) \leq m(n-2)<0.5 n^{3}
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$$

- $G$ is distance-balanced if $n_{G}(u, v)=n_{G}(v, u)$ for every edge $u v$ of $G$.


## Mostar index

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|  | Contents lists available at ScienceDirect <br> Applied Mathematics and Computation |  |
| :---: | :---: | :---: |

Mostar index: Results and perspectives

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## ABSTRACT

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.

## Relation to the Wiener index

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

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

Since

$$
\left|n_{G}(u, v)-n_{G}(v, u)\right|=\left|\sigma_{G}(u)-\sigma_{G}(v)\right| \text { for every edge } u v \text { of } G,
$$

we have

$$
\operatorname{Mo}(G)=\sum_{u v \in E(G)}\left|\sigma_{G}(u)-\sigma_{G}(v)\right| .
$$

## Relation to the irregularity

The irregularity $\operatorname{irr}(G)$ of a graph $G$ [Albertson 1997] is

$$
\operatorname{irr}(G)=\sum_{u v \in E(G)}\left|d_{G}(u)-d_{G}(v)\right| .
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$$

If $\operatorname{diam}(G) \leq 2$, then


$$
\begin{aligned}
\left|n_{G}(u, v)-n_{G}(v, u)\right| & =|(a+1)-(c+1)| \\
& =|(a+b+1)-(b+c+1)| \\
& =\left|d_{G}(u)-d_{G}(v)\right|
\end{aligned}
$$

and, hence,

$$
M o(G)=\operatorname{irr}(G)
$$

## Two conjectures from [Doslic et al. 2018]

### 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 $\operatorname{Mo}(G) \neq 0$.

We have already mentioned that $\operatorname{Mo}\left(K_{\lfloor n / 3\rfloor,\lceil 2 n / 3\rceil}\right) \sim 2 n^{3} / 27 \in \Theta\left(n^{3}\right)$. 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 $K_{n / 3,2 n / 3}$ 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 $S_{n / 3,2 n / 3}$ has the maximal Mostar index.

Two conjectures from [Doslic et al. 2018]
As observed by Geneson and Tsai [2021], for $\alpha \leq \frac{1}{2}$,

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

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 $n$,

$$
M o\left(K_{0.211 \ldots n, 0.789 \ldots n}\right)>\operatorname{Mo}\left(K_{0 . \overline{3} n, 0 . \overline{6} n}\right),
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$$

and Conjecture 19 cannot hold as stated.
Albertson [1997] showed

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

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

## Bipartite graphs

## Theorem (MPRW 2022)

If $G$ is a bipartite graph of order $n$, then

$$
\operatorname{Mo}(G) \leq \alpha^{\star}\left(1-\alpha^{\star}\right)\left(1-2 \alpha^{\star}\right) n^{3}=\frac{\sqrt{3}}{18} n^{3} \approx 0.096225 n^{3}
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For an edge $u v$ of a bipartite graph $G$, we have

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$$

which implies

$$
\begin{aligned}
\left|n_{G}(u, v)-n_{G}(v, u)\right| & \leq n-2 \min \left\{d_{G}(u), d_{G}(v)\right\} \\
& =n\left(1-\frac{2}{n} \min \left\{d_{G}(u), d_{G}(v)\right\}\right) .
\end{aligned}
$$

## Bipartite graphs

We obtain

$$
M o(G) \leq \sum_{u v \in E(G)} n\left(1-\frac{2}{n} \min \left\{d_{G}(u), d_{G}(v)\right\}\right)
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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 $\alpha n$ and $(1-\alpha) n$ for some $\alpha \in(0,1 / 2]$.


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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 $j \in J$.


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- 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 $(i, j) \in I \times J$.


## Bipartite graphs

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

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

$$
\sum_{j \in J} m_{i, j}-\frac{i x_{i}}{(1-\alpha) n}=0 \text { for every } i \in I
$$

and, symmetrically,

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

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\begin{aligned}
& \sum_{i \in I} m_{i, j}-\frac{j y_{j}}{\alpha n}=0 \text { for every } j \in J . \\
M o(G) & \leq \sum_{u v \in E(G)} n\left(1-\frac{2}{n} \min \left\{d_{G}(u), d_{G}(v)\right\}\right) \\
& =\left(\sum_{(i, j) \in I \times J} m_{i, j}\left(1-\frac{2}{n} \min \{i, j\}\right)\right) \alpha(1-\alpha) n^{3} .
\end{aligned}
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We obtain

$$
\operatorname{Mo}(G) \leq \operatorname{OPT}(P) \alpha(1-\alpha) n^{3}
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for the following linear programm $(P)$ :

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for the following linear programm $(P)$ :

$$
\max \sum_{(i, j) \in I \times J} m_{i, j}\left(1-\frac{2}{n} \min \{i, j\}\right),
$$

s.th.

$$
\begin{aligned}
\sum_{i \in I} x_{i} & =1 \\
\sum_{j \in J} y_{j} & =1 \\
\sum_{j \in J} m_{i, j}-\frac{i x_{i}}{(1-\alpha) n} & =0 \quad \text { for every } i \in I \\
\sum_{i \in I} m_{i, j}-\frac{j y_{j}}{\alpha n} & =0 \quad \text { for every } j \in J \\
x_{i}, y_{j}, m_{i, j} & \geq 0 \quad \text { for every }(i, j) \in I \times J .
\end{aligned}
$$

## Bipartite graphs

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

$$
\begin{array}{rlrl}
\min & p+q, & & \\
\text { s.th. } & p_{i}+q_{j} & \geq 1-\frac{2}{n} \min \{i, j\} & \\
\text { for every } i \in I \text { and every } j \in J,  \tag{D}\\
p & \geq \frac{i p_{i}}{(1-\alpha) n} & & \text { for every } i \in I, \\
q & \geq \frac{j q_{j}}{\alpha n} & & \text { for every } j \in J, \\
p, q, p_{j}, q_{j} & \in \mathbb{R} & & \text { for every } i \in I \text { and every } j \in J .
\end{array}
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p & & \text { for every } i \in I \text { and every } j \in J, \\
p & \geq \frac{i p_{i}}{(1-\alpha) n} & & \text { for every } i \in I, \\
q & \geq \frac{j q_{j}}{\alpha n} & & \text { for every } j \in J, \\
p, q, p_{j}, q_{j} & \in \mathbb{R} & & \text { for every } i \in I \text { and every } j \in J .
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p & \geq \frac{i p_{i}}{(1-\alpha) n} & & \text { for every } i \in I, \\
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p, q, p_{j}, q_{j} & \in \mathbb{R} & & \text { for every } i \in I \text { and every } j \in J .
\end{array}
$$

- We just need weak duality $\operatorname{OPT}(P) \leq \operatorname{OPT}(D)$.
- $p \stackrel{!}{=} \frac{i p_{i}}{(1-\alpha) n}$ for $i \geq 1 \Rightarrow p_{i}=\frac{(1-\alpha) n}{i} p$.
- $q_{j}=\frac{\alpha n}{j} q$ for $j \geq 1$.


## Bipartite graphs

$$
p_{i}+q_{j} \geq 1-\frac{2}{n} \min \{i, j\} \text { for } 1 \leq i \leq j
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\Uparrow \\
\frac{p}{\left(\frac{i}{(1-\alpha) n}\right)}+\frac{2 i}{n}+q \geq 1 \text { for } 1 \leq i \leq \alpha n .
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\frac{p}{\left(\frac{i}{(1-\alpha) n}\right)}+\frac{2 i}{n}+q \geq 1 \text { for } 1 \leq i \leq \alpha n . \\
\Uparrow \\
\left(\frac{p}{x}+2(1-\alpha) x\right)+q \geq 1 \quad \text { for } \quad x=\frac{i}{(1-\alpha) n} \in\left(0, \frac{\alpha}{1-\alpha}\right] .
\end{gathered}
$$

## Bipartite graphs



For some $\delta>0$, the function

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

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

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

## Bipartite graphs

It follows $\operatorname{OPT}(D) \leq \operatorname{OPT}\left(D^{\prime}\right)$ for

$$
\min \quad p+q,
$$

$$
\text { s.th. } \quad p+q \geq 1-2 \alpha
$$

( $D^{\prime}$ )

$$
\begin{aligned}
p+2 \sqrt{2 q \alpha} & \geq 1 & \text { if } q<2 \alpha \\
2 \sqrt{2 p(1-\alpha)}+q & \geq 1 & \text { if } p<\frac{2 \alpha^{2}}{1-\alpha} \\
p, q & \geq 0 . &
\end{aligned}
$$

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

The proof is now completed by showing

$$
\operatorname{OPT}\left(D^{\prime}\right) \leq \frac{\alpha^{\star}\left(1-\alpha^{\star}\right)\left(1-2 \alpha^{\star}\right)}{\alpha(1-\alpha)}
$$

Split graphs

## Split graphs

## Theorem (MPRW 2022)

If $G$ is a split graph that arises from a clique $C$ of order $\alpha n$ 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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$$
\left.\begin{array}{rl}
\operatorname{Mo}(G) & \leq((1+\alpha) n-1) m-\frac{2 m^{2}}{(1-\alpha) n} \\
& \leq\left\{\begin{array}{ll}
\alpha(1-\alpha) n^{2}((1-\alpha) n-1) & , \text { if } \alpha \leq \frac{1}{3}-\frac{1}{3 n} \\
\frac{1}{8}(1-\alpha) n((1+\alpha) n-1)^{2}
\end{array}, \text { if } \alpha>\frac{1}{3}-\frac{1}{3 n}\right.
\end{array}\right] \begin{aligned}
& \\
&
\end{aligned}
$$

Each stated bound is best possible up to $O\left(n^{2}\right)$.

## Split graphs

Let $G$ be as in the statement and let $u v$ be an edge of $G$.

$$
\left|n_{G}(u, v)-n_{G}(v, u)\right| \leq \begin{cases}n-d_{G}(v)-1 & , \text { if } u \in C \text { and } v \in I \\ \left|d_{G}(u)-d_{G}(v)\right| & , \text { if } u, v \in C\end{cases}
$$

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

## Split graphs

Let $G$ be as in the statement and let $u v$ be an edge of $G$.

$$
\left|n_{G}(u, v)-n_{G}(v, u)\right| \leq \begin{cases}n-d_{G}(v)-1 & , \text { if } u \in C \text { and } v \in I \\ \left|d_{G}(u)-d_{G}(v)\right| & , \text { if } u, v \in C\end{cases}
$$

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

$$
\begin{aligned}
\operatorname{Mo}(G) & \leq \sum_{u v \in E}\left(n-d_{G}(v)-1\right)+\sum_{u v \in\binom{c}{2}}\left|d_{G}(u)-d_{G}(v)\right| \\
& =m(n-1)-\sum_{v \in I} d_{G}(v)^{2}+\sum_{u v \in\binom{c}{2}}\left|d_{G}(u)-d_{G}(v)\right| \\
& \leq m(n-1)-\frac{m^{2}}{(1-\alpha) n}+\sum_{u v \in\binom{c}{2}}\left|d_{G}(u)-d_{G}(v)\right| \\
& \leq m(n-1)-\frac{m^{2}}{(1-\alpha) n}+\alpha n m-\frac{m^{2}}{(1-\alpha) n}
\end{aligned}
$$

## General graphs

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Conjecture 20 would imply

$$
M o(G) \leq \frac{4}{27} n^{3}=0 . \overline{148} n^{3}
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Geneson and Tsai [2021] improved $\operatorname{Mo}(G)<0.5 n^{3}$ to

$$
\begin{aligned}
M o(G) \leq M o^{\star}(G) & :=\sum_{u v \in E(G)} \underbrace{\left(n-\min \left\{d_{G}(u), d_{G}(v)\right\}\right)}_{\geq\left|n_{G}(u, v)-n_{G}(v, u)\right|} \\
& \leq \frac{5}{24}(1+o(1)) n^{3} \approx 0.2083(1+o(1)) n^{3} .
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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
$M o^{\star}(G) \leq\left(2\left(\frac{\Delta}{n}\right)^{2}+\left(\frac{\Delta}{n}\right)-2\left(\frac{\Delta}{n}\right) \sqrt{\left(\frac{\Delta}{n}\right)^{2}+\left(\frac{\Delta}{n}\right)}\right) n^{3} \leq(3-2 \sqrt{2}) n^{3} \approx 0.1716 n^{3}$.

## General graphs

## Theorem (MPRW 2022)

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

## General graphs

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## General graphs

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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) $M o^{\star}(G)$ 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.

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There is a linear ordering $\pi: u_{1}, u_{2}, \ldots, u_{n}$ of $V(G)$ such that

$$
d_{G}\left(u_{1}\right) \leq d_{G}\left(u_{2}\right) \leq \ldots \leq d_{G}\left(u_{n}\right)
$$

and

$$
d_{1}^{+} \geq d_{2}^{+} \geq \ldots \geq d_{n}^{+}
$$

where $d_{i}^{+}$be the number of forward edges at $u_{i}$.

## General graphs

$\delta=d_{G}\left(u_{1}\right)$.

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$u_{1}$

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$\delta=d_{G}\left(u_{1}\right)$.
$u_{1}$
$u_{n-\delta}$

General graphs
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$$
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$n-\min \left\{d_{G}(u), d_{G}(v)\right\}=\delta-\min \left\{d_{H}(u), d_{H}(v)\right\}$ for every edge $u v$ of $H$

## General graphs

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$n-\min \left\{d_{G}(u), d_{G}(v)\right\}=\delta-\min \left\{d_{H}(u), d_{H}(v)\right\}$ for every edge $u v$ of $H$

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

Irregularity

Irregularity

Albertson [1997] defined the irregularity $\operatorname{irr}(G)$ of a graph $G$ as

$$
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$$

Irregularity

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\operatorname{irr}(G)=\sum_{u v \in E(G)}\left|d_{G}(u)-d_{G}(v)\right| \\
\operatorname{irr}(G \pm e) \leq \operatorname{irr}(G) \forall e \Rightarrow G=S_{p, n-p}=K_{p} \circ \bar{K}_{n-p}
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\operatorname{irr}(G \pm e) \leq \operatorname{irr}(G) \forall e \Rightarrow G=S_{p, n-p}=K_{p} \circ \bar{K}_{n-p} \\
\operatorname{irr}(G) \leq \max _{p} S_{p, n-p}=\left\lfloor\frac{n}{3}\right\rfloor\left\lceil\frac{2 n}{3}\right\rceil\left(\left\lceil\frac{2 n}{3}\right\rceil-1\right)<\frac{4 n^{3}}{27}
\end{gathered}
$$

Irregularity

Hansen and Mélot [2005]

$$
\operatorname{irr}(G) \leq f(n, m)
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## Irregularity

For a graph $G$ with $n$ vertices, $m$ edges, maximum degree $\Delta$, and minimum degree $\delta$, Zhou and Luo [2008] showed

$$
\begin{aligned}
& \operatorname{irr}(G) \leq m \sqrt{\frac{2 n(2 m+(n-1)(\Delta-\delta))}{n+\Delta-\delta}-4 m} \\
& \operatorname{irr}(G) \leq \sqrt{m\left(2 m n(\Delta+\delta)-n^{2} \Delta \delta-4 m^{2}\right)}
\end{aligned}
$$

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]

The irregularity of a graph of bounded maximum degree

The irregularity of a graph of bounded maximum degree

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

## Theorem (RW 2023)

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

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

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



The irregularity of a graph of bounded maximum degree

## Corollary (RW 2023)

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

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




The irregularity of a graph of bounded maximum degree
Comparing to Zhou and Luo [2008]:


The irregularity of a graph of bounded maximum/minimum degree

The irregularity of a graph of bounded maximum/minimum degree For integers $\Delta>\delta \geq 0$, let

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

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

## Proposition (RW 2023)

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

$$
\operatorname{irr}(G) \leq \frac{\Delta\left(\Delta-\delta^{*}\right) \delta^{*}}{\Delta+\delta^{*}} n .
$$

The irregularity of a graph of bounded maximum/minimum degree

## Proposition (RW 2023)

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

$$
\operatorname{irr}(G) \leq 2 \Delta m-\delta \Delta n
$$

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


## Proofs

## Proofs

Let $I_{0}=\{0,1, \ldots, \Delta\}$ and $I=I_{0} \backslash\{0\}$.

$$
\operatorname{irr}(G) \leq \mathrm{OPT}(P)
$$

max

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

s.th.
( $P$ )

$$
\begin{aligned}
& \sum_{i \in I_{0}} n_{i}=n \\
& \sum_{i \in I} i n_{i}=2 m
\end{aligned}
$$

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

$$
n_{i} \in \mathbb{R}_{\geq 0} \quad \text { for every } i \in I_{0}, \text { and }
$$

$$
m_{i, j} \in \mathbb{R}_{\geq 0} \quad \text { for every } i, j \in I \text { with } i \leq j
$$

## Proofs

$$
\begin{array}{rlll}
\min & n x+2 m y & & \\
\text { s.th. } & z_{i}+z_{j} & \geq j-i & \text { for every } i, j \in I \text { with } i<j, \\
x+i y & \geq i z_{i} & \text { for every } i \in I,  \tag{D}\\
x & \in \mathbb{R}_{\geq 0}, & \\
y & \in \mathbb{R}^{2} & \text { and } \\
z_{i} & \in \mathbb{R}_{\geq 0}, \quad \text { for every } i \in I .
\end{array}
$$

## Proofs

$$
\begin{aligned}
& \min n x+2 m y \\
& \text { s.th. } \quad z_{i}+z_{j} \geq j-i \quad \text { for every } i, j \in I \text { with } i<j \text {, } \\
& \text { (D) } \\
& \begin{aligned}
x+i y & \geq i z_{i} \\
x & \in \mathbb{R}_{\geq 0},
\end{aligned} \\
& y \in \mathbb{R} \text {, and } \\
& z_{i} \in \mathbb{R}_{\geq 0}, \quad \text { for every } i \in I . \\
& \sum_{i, j \in 1: i<j}(j-i) m_{i, j} \\
& \leq \sum_{i, j \in I: i<j}(\underbrace{z_{i}+z_{j}}_{\geq j-i}) m_{i, j}+\underbrace{2 \sum_{i \in I} z_{i} m_{i, i}+x n_{0}+\sum_{i \in I}\left(x+i y-i z_{i}\right) n_{i}}_{\geq 0} \\
& =\left(\sum_{i \in I_{0}} n_{i}\right) x+\left(\sum_{i \in I} i n_{i}\right) y+\sum_{i \in I}\left(2 m_{i, i}+\sum_{j \in I: j<i} m_{j, i}+\sum_{j \in I: j>i} m_{i, j}-i n_{i}\right) z_{i} \\
& =n x+2 m y \text {. }
\end{aligned}
$$

## Proofs

$\left(x, y,\left(z_{i}\right)_{i \in I}\right)$ with

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

is a feasible solution for $(D)$.

## Proofs

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

is a feasible solution for $(D)$.

$$
\begin{aligned}
\operatorname{irr}(G) & \leq \operatorname{OPT}(P) \\
& \leq \operatorname{OPT}(D) \\
& \leq n x+2 m y \\
& =d(d+1) n+\frac{1}{\Delta}\left(\Delta^{2}-(2 d+1) \Delta-d^{2}-d\right) m
\end{aligned}
$$

A problem from [Doslic et al. 2018]

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

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

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

We conjecture that

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

is

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

## A problem from [Doslic et al. 2018]

## Theorem (HPRW 2023)

For integers $n_{0}$ and $\Delta$ at least 3 , there is a $\Delta$-regular graph $G$ of order $n$ at least $n_{0}$ with

$$
M o(G) \geq \frac{\Delta}{2} n^{2}-\left(20 \Delta^{3}+12 \Delta^{2}-24 \Delta+48\right) n \log _{(\Delta-1)}(n) .
$$

A problem from [Doslic et al. 2018]

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## Theorem (HPRW 2023)

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

$$
M o(G) \leq \frac{\Delta}{2} n^{2}-(2-o(n)) \frac{(\Delta-2)}{(\Delta-1)^{2}} n \log _{(\Delta-1)}\left(\log _{(\Delta-1)}(n)\right)
$$

A problem from [Doslic et al. 2018]


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$$
\begin{aligned}
\left|n_{G}(u, v)-n_{G}(v, u)\right| & \leq n-2 \min \{p, q\} \\
\sum_{u v \in E(T)} \min \{p, q\} & \geq(1-o(n)) c_{\Delta} n \log (\log (n))
\end{aligned}
$$

Thank you for the attention!


